



# Probabilistic global-local calibration of crystal plasticity parameters for additively manufactured metals using synthetic data

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<sup>3</sup>Science and Technology Corporation

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# Outline

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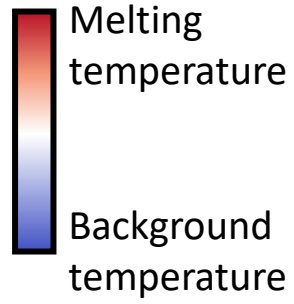
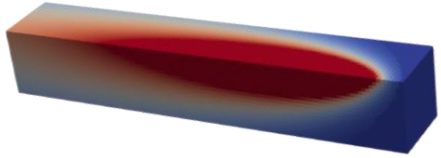


- Motivation
  - Additive manufacturing (AM) simulations
  - Calibration, validation, and uncertainty quantification (UQ) challenges
- Crystal plasticity
- Sensitivity study
- Calibration approach and results
- Conclusions and outlook

# Motivation: AM simulations

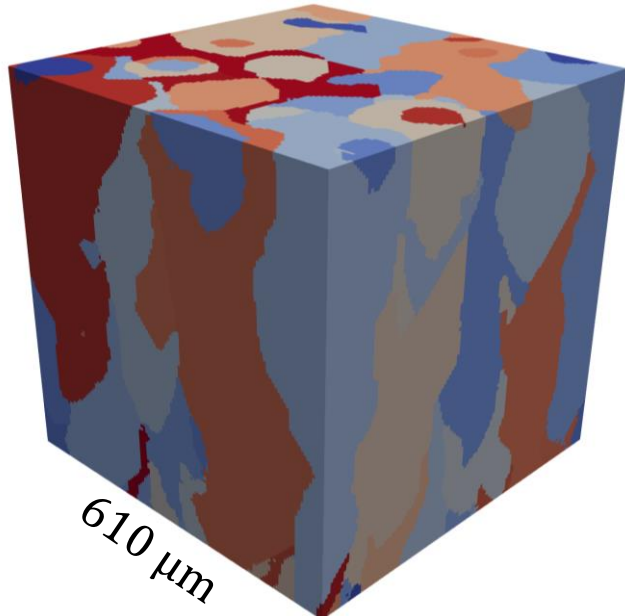


1. Thermal model: melt pool, temperature field

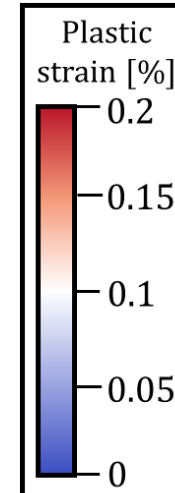
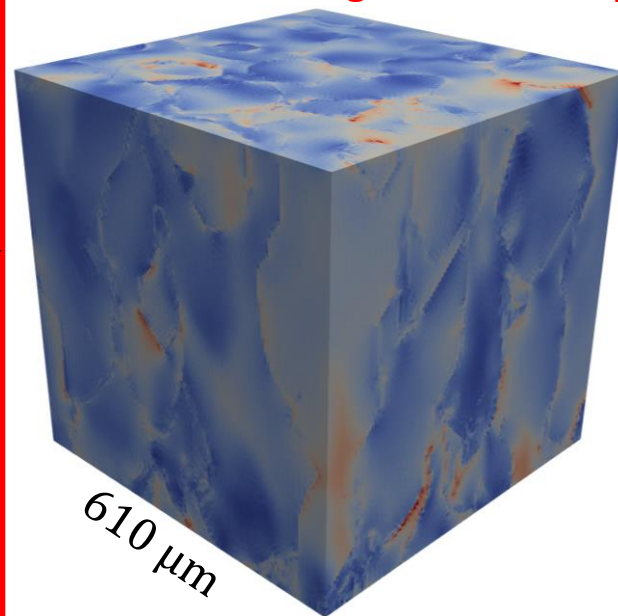


- Process-structure-property simulations: understand how AM process changes/variations influence mechanical behavior
- Goals: accelerate design iterations, help with process parameter selection, augment qualification and certification processes
- Here: case study using a crystal plasticity model

2. Process-structure model: solidification, texture, defects



3. Structure-property model: stress and strain fields, fatigue indicator parameters



J.D. Pribe, B. Richter, P.E. Leser, S.R. Yeratapally, G.R. Weber, A.R. Kitahara, E.H. Glaessgen, "A process-structure-property simulation framework for quantifying uncertainty in additive manufacturing: Application to fatigue in Ti-6Al-4V", *Integr Mater Manuf Innov* 12 (2023) 231–250.

<https://doi.org/10.1007/s40192-023-00303-9>

# Motivation: Calibration, validation, and UQ challenges



- Crystal plasticity → fatigue crack initiation and microstructurally small crack growth predictions
- Problem: complex interaction of assumptions and limitations in crystal plasticity

**What physics to incorporate? At what length scale(s)?**

**What calibration data is available? At what length/time scale(s)? Global stress-strain data, HEDM, DIC, ...**

**What is known about the microstructure? At what length scale(s)?**

**How to achieve calibration, validation, and UQ with computational cost constraints?**

**Can others reproduce the same results?**

# Motivation: Calibration, validation, and UQ challenges

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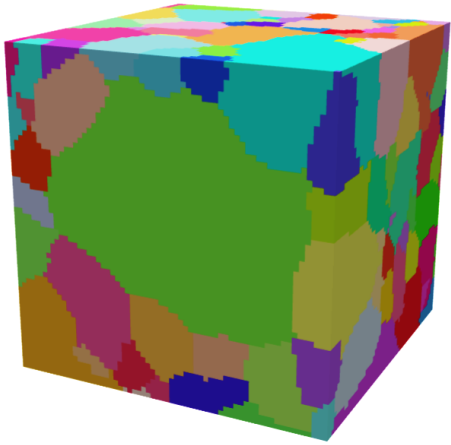
**Given synthetic calibration data from the ground-truth crystal plasticity model...**

- To what extent does probabilistic calibration recover the true parameters?
- What is the influence of data from different experimental modalities?
- What inferences can be made about “real” problems?

# Methods overview



IN 718 microstructure



1000 simulations with samples from calibration parameters

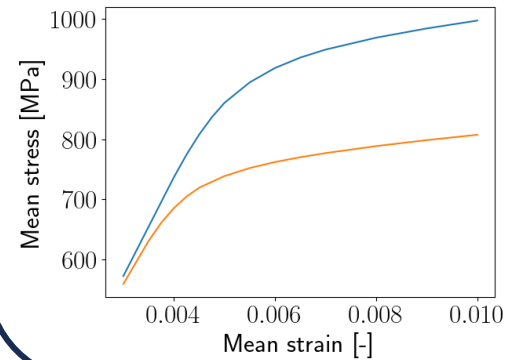
- Rate sensitivity, initial CRSS, hardening coefficient, dynamic recovery coefficient

Fast Fourier transform (FFT)  
crystal plasticity solver

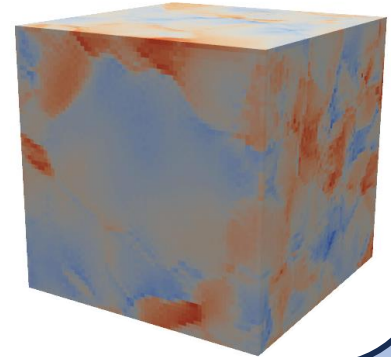
CRSS: critical resolved shear stress

Sensitivity study on calibration parameters

Stress-strain curve



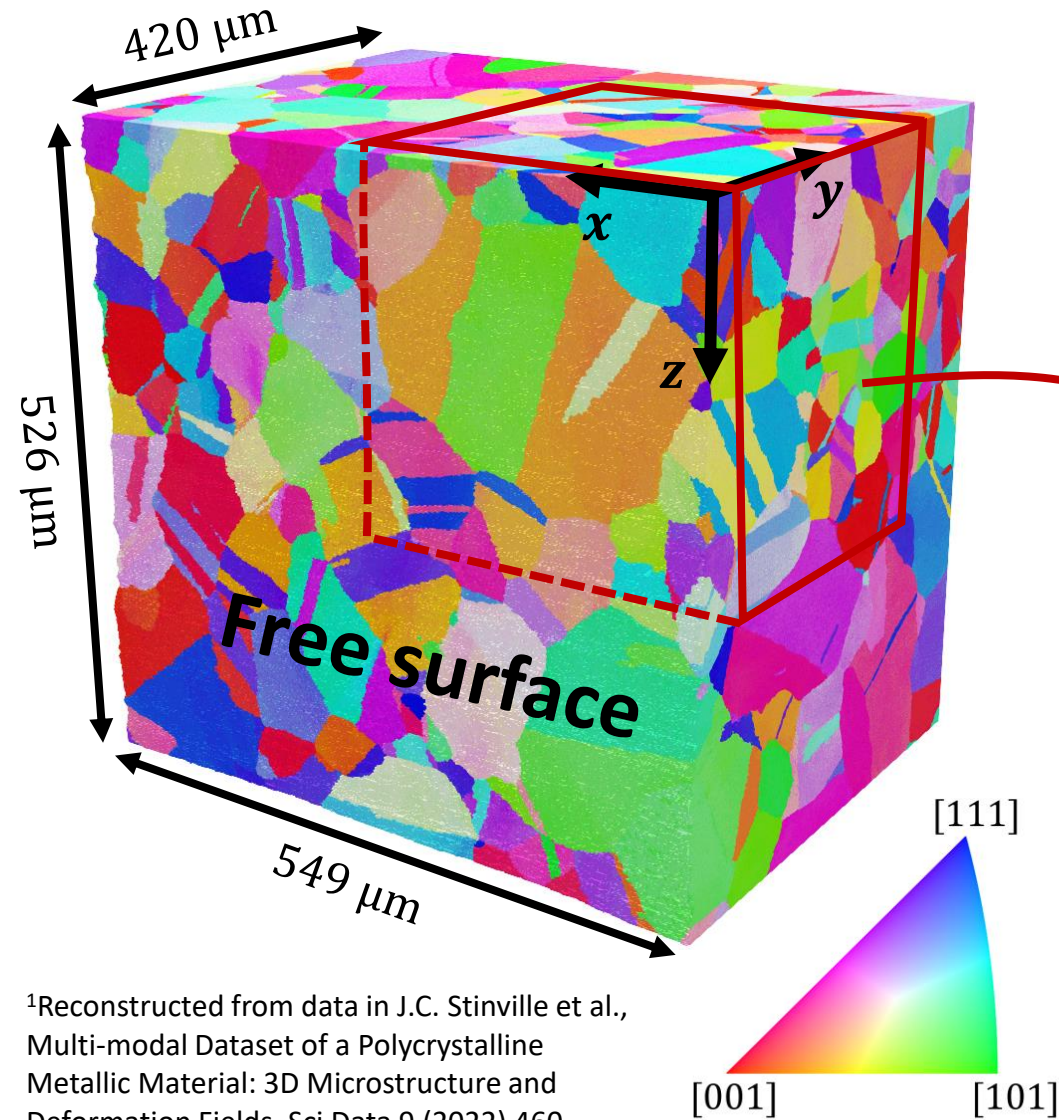
Local stresses



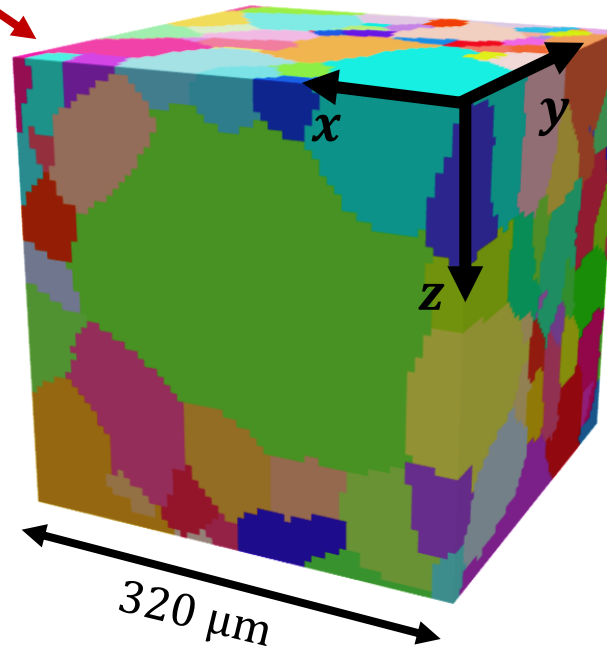
# Crystal plasticity: Microstructure

Inverse pole figure (IPF) map in x direction<sup>1</sup>

- 3-D Inconel 718 microstructure from open-source dataset<sup>1</sup>
- Simplify for simulations (surfaces, discretization, twins, domain size)



IPF map of simplified microstructure (64 × 64 × 64 voxels)

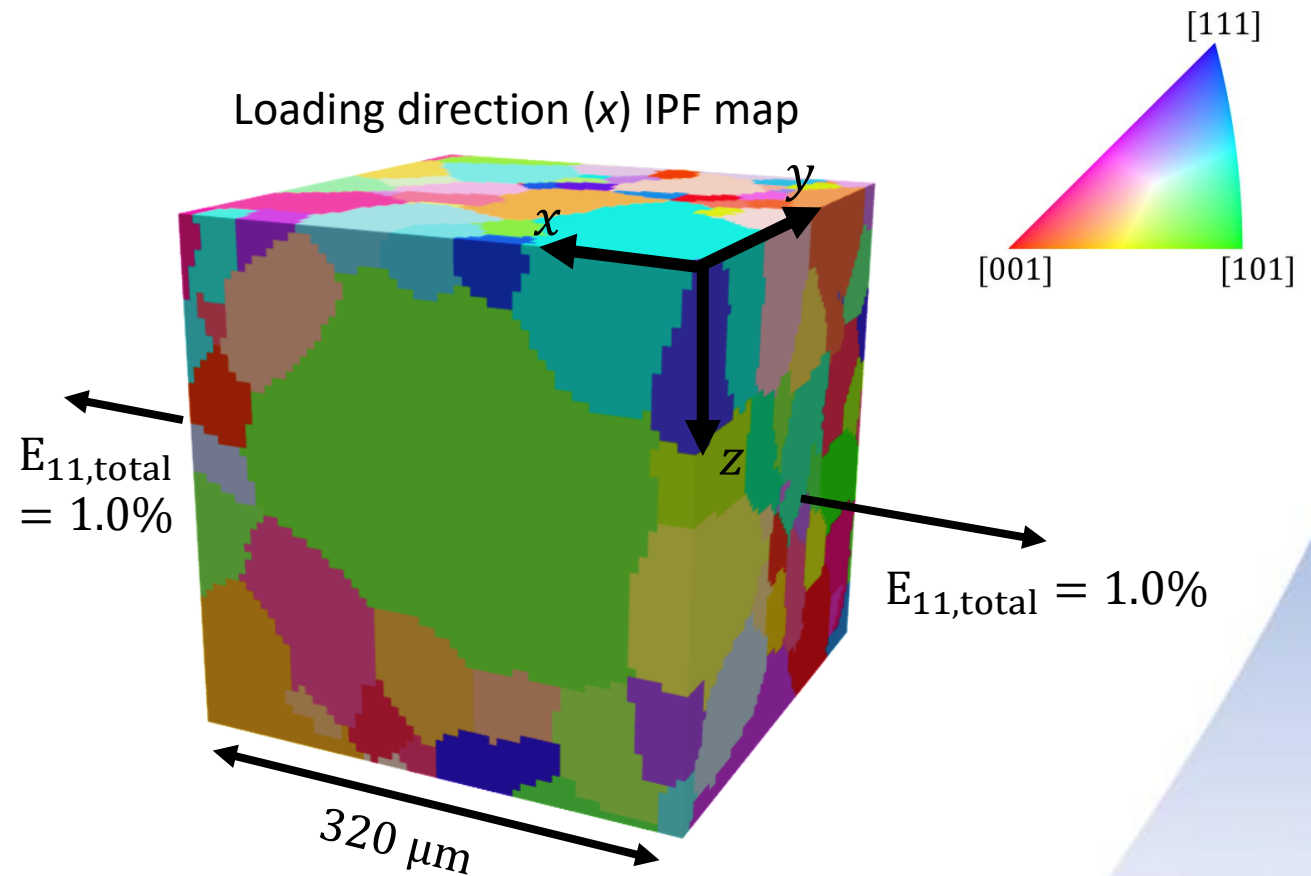


<sup>1</sup>Reconstructed from data in J.C. Stinville et al., Multi-modal Dataset of a Polycrystalline Metallic Material: 3D Microstructure and Deformation Fields, Sci Data 9 (2022) 460

# Crystal plasticity: Simulation methods



- FFT-based crystal plasticity solver<sup>1,2</sup>
  - Generally faster than finite elements
  - Well-suited for voxelized domains
- Applied loading
  - Uniaxial strain in x direction
  - Mean stress = 0 for all other components



<sup>1</sup>J. Zeman et al., A finite element perspective on nonlinear FFT-based micromechanical simulations, Int J Numer Meth Engr 111 (2017) 903–926. <https://doi.org/10.1002/nme.5481>.

<sup>2</sup>T.W.J. de Geus et al., Finite strain FFT-based non-linear solvers made simple, Comput Methods Appl Mech Eng 318 (2017) 412–430. <https://doi.org/10.1016/j.cma.2016.12.032>.

# Crystal plasticity: Simulation methods

- Goal: use a simple constitutive model that still has interesting behavior
- Calibration parameters in red

Viscoplastic flow rule

$$\dot{\gamma}_s = \dot{\gamma}_0 \left| \frac{\tau_s}{g_s} \right|^m \text{sgn } \tau_s$$

$\dot{\gamma}_s$ : slip rate on slip system  $s$

$\dot{\gamma}_0$ : reference slip rate

$\tau_s$ : shear stress on slip system  $s$

$g_s$ : CRSS for slip system  $s$

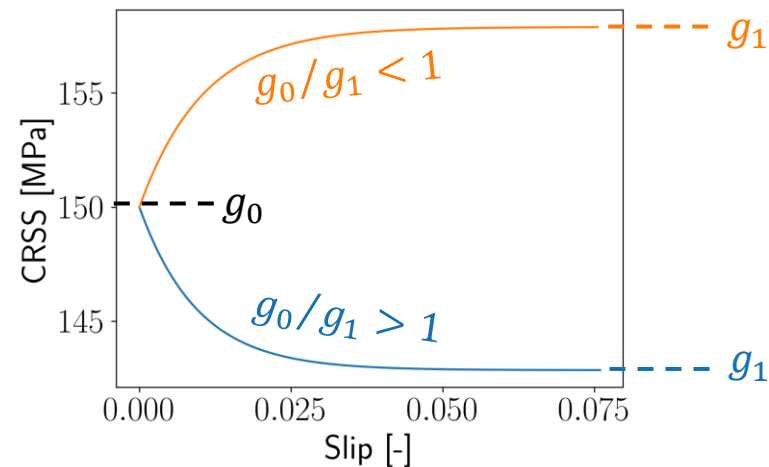
$m$ : rate sensitivity exponent

Armstrong-Frederick hardening

$$\begin{aligned} \dot{g}_s &= (H - H_d g_s) \dot{\Gamma} && \text{Assume self and latent} \\ g_s &= g_0 + \int_0^t \dot{g}_s dt && \text{hardening constants are unity} \end{aligned}$$

Saturation stress:  $g_1 = g_s(\dot{g}_s = 0) = H/H_d$

Example hardening and softening behavior



$g_0$ : initial CRSS on all slip systems

$H$ : hardening coefficient

~~$H_d$ : dynamic recovery coefficient~~

$g_0/g_1$ : CRSS ratio

# Sensitivity study



Inputs:

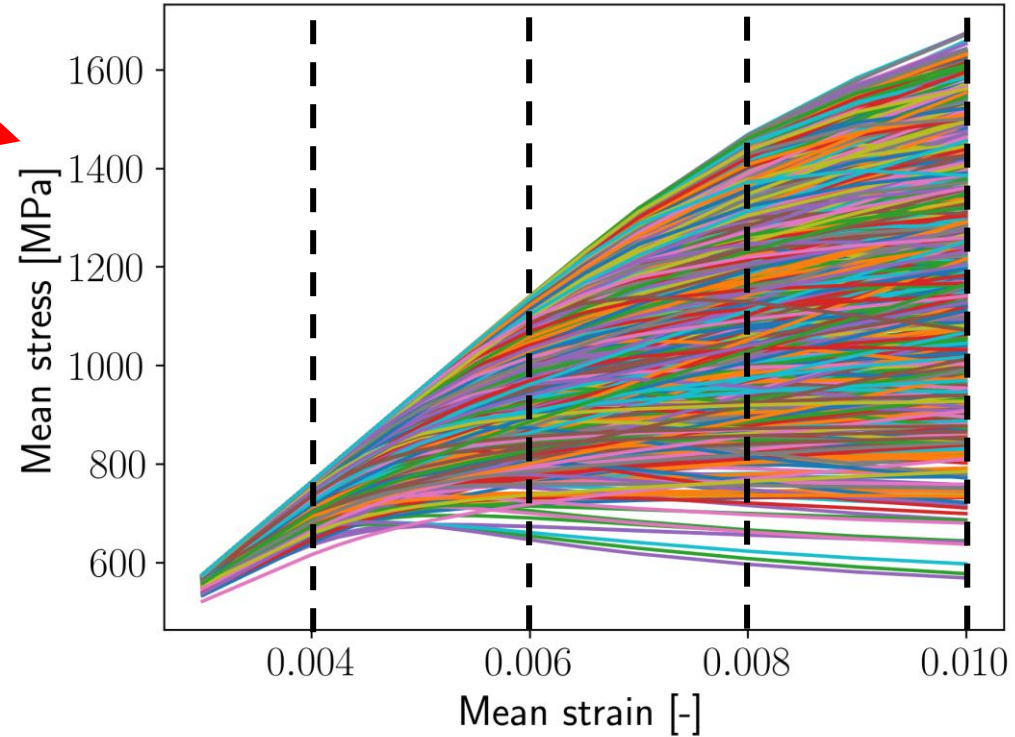
1000 samples

- $5 \leq m \leq 30$
- $300 \text{ MPa} \leq g_0 \leq 700 \text{ MPa}$
- $1000 \text{ MPa} \leq H \leq 30000 \text{ MPa}$
- $0 \leq \frac{g_0}{g_1} \leq 1.5$

Outputs to consider:

- Mean (global) stresses at four mean strain values in the plastic regime

Stress-strain curves in plastic regime



# Sensitivity study

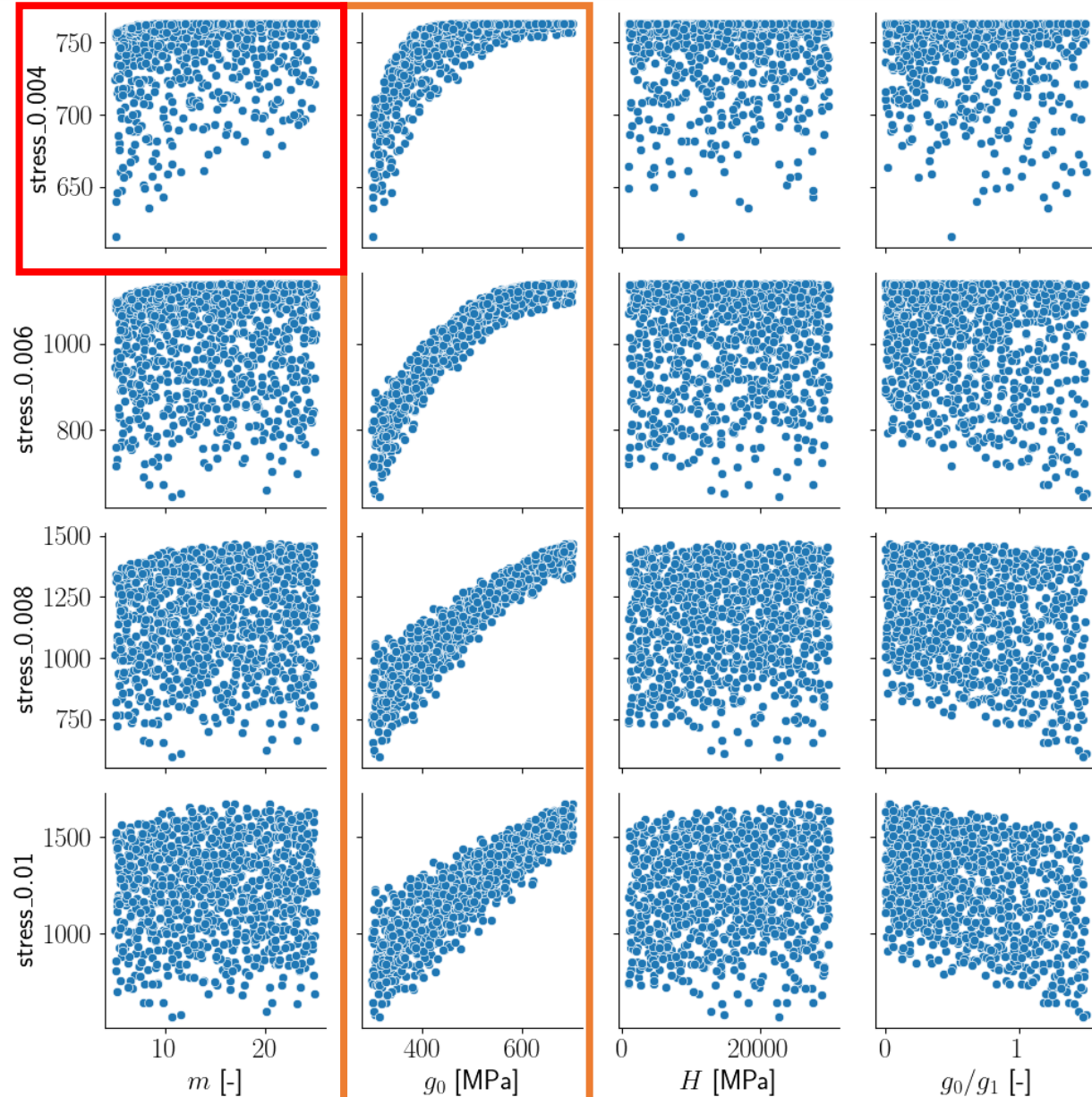


Pair plots (joint distributions) of mean stresses with calibration parameters

- Stresses are generally correlated with initial CRSS
- Low yield point is also correlated with low  $m$  (higher rate sensitivity)



Increasing applied strain



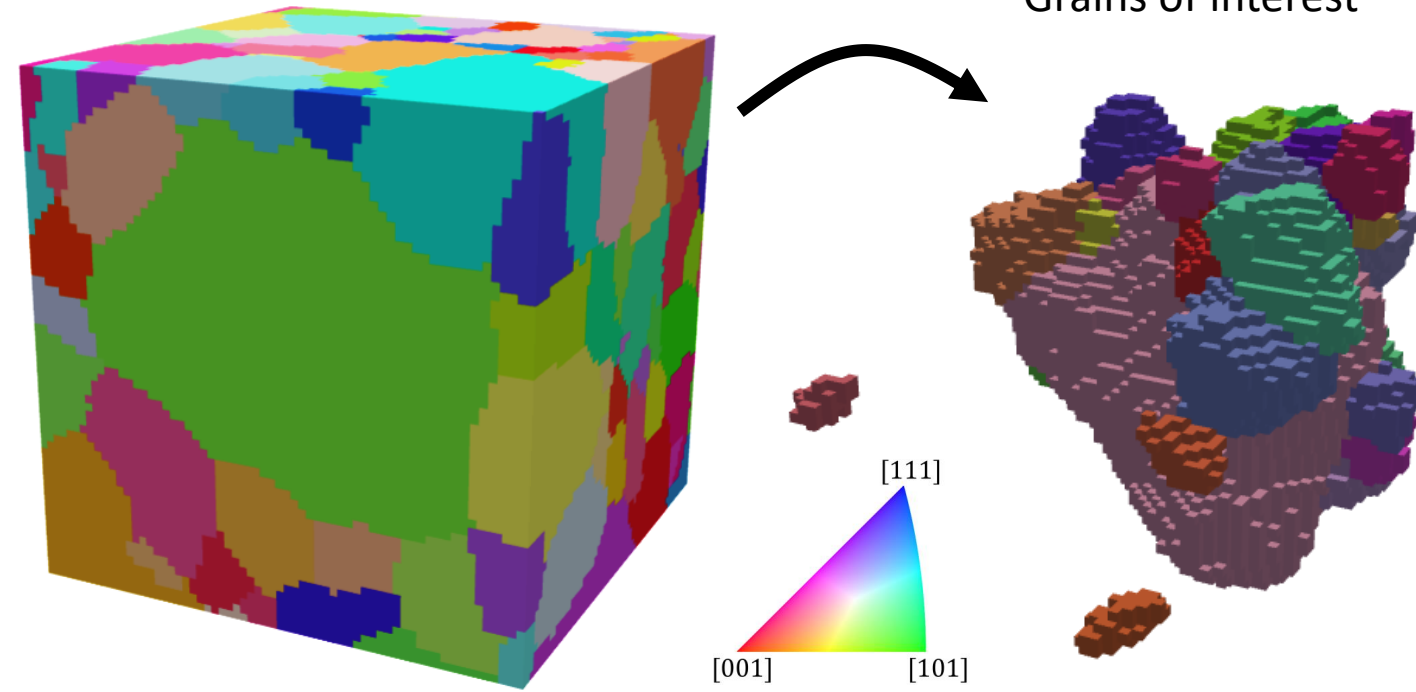
# Sensitivity study



Outputs to consider:

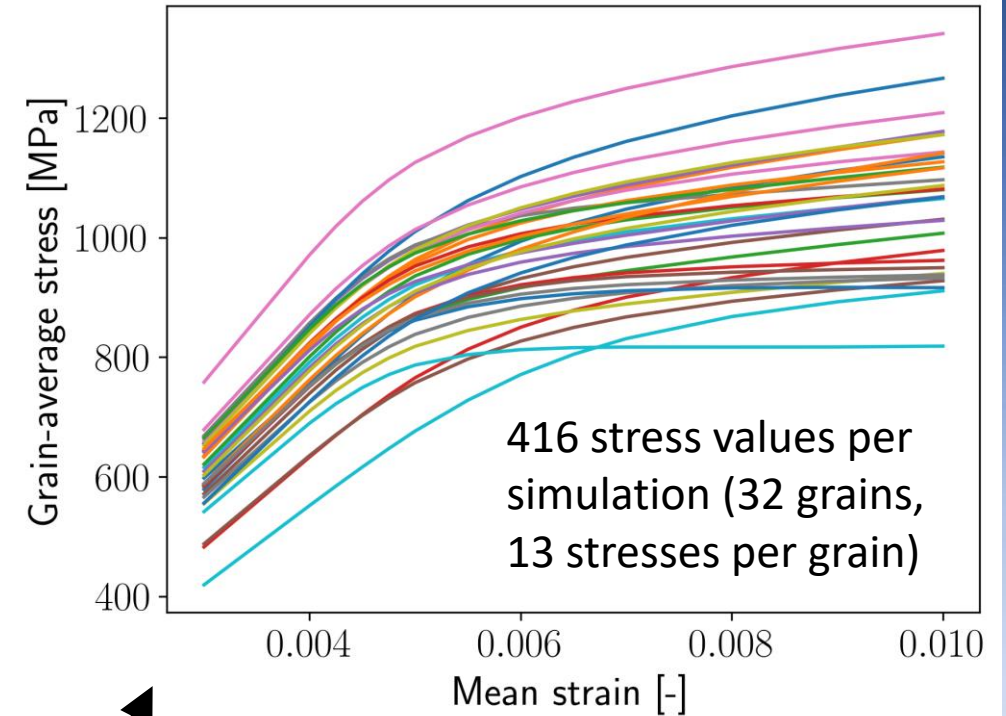
- Mean (global) stresses
- Grain-average stresses for 32 grains
  - At least 20 voxels in volume
  - At least 5 voxels from a “surface”

Grains of interest



1000 samples

Grain-average stresses for one example simulation

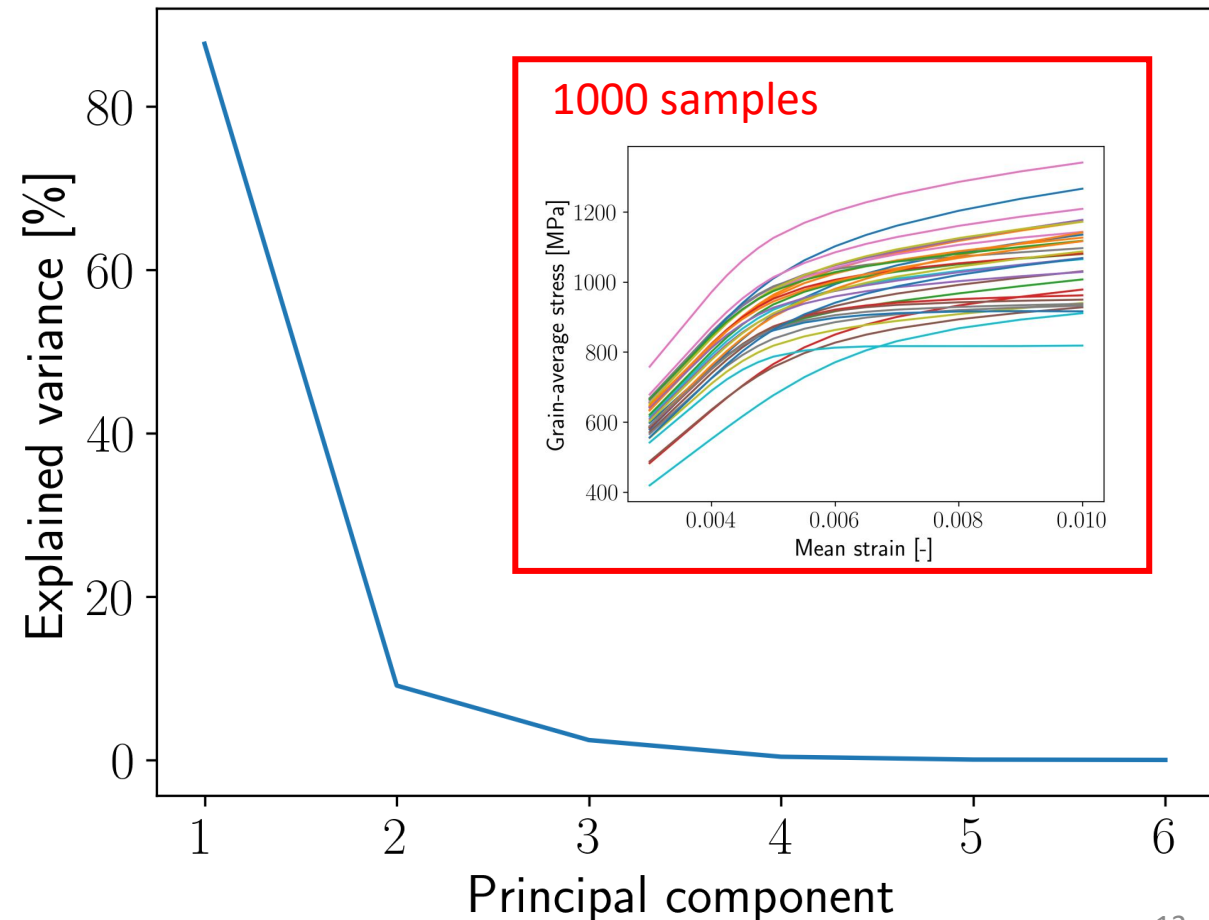


# Sensitivity study

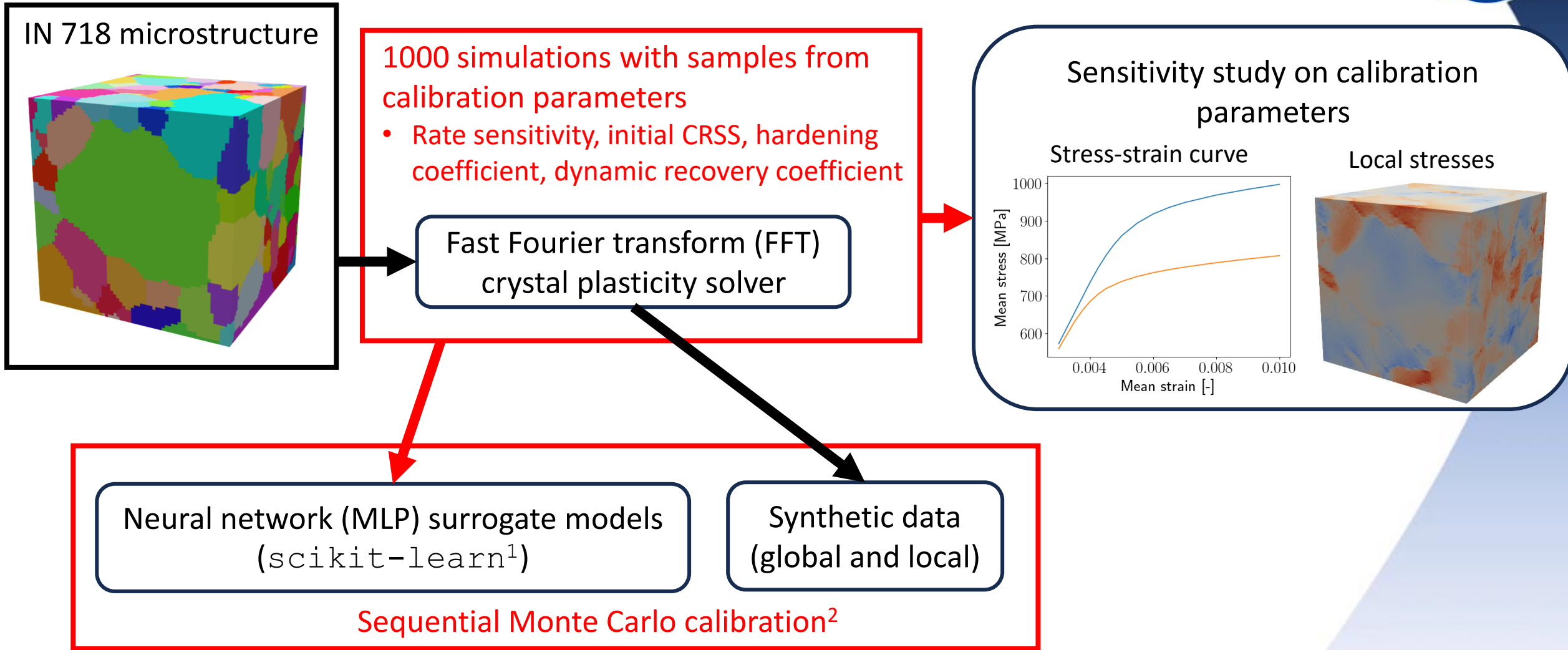


- Dimensionality reduction with principal component analysis (PCA)
- 1 PC explains ~85% of the variance
  - Remaining PCs are all <10%
- First PC is strongly correlated with initial CRSS → calibration challenges even with local data

Explained variance for principal components (PCs) of grain-average stresses



# Methods overview



CRSS: critical resolved shear stress    MLP: multi-layer perceptron

<sup>1</sup>F. Pedregosa et al., Scikit-learn: Machine Learning in Python, JMLR 12 (2011) 2825–2830.

<sup>2</sup><https://github.com/nasa/SMCPy>

# Calibration approach

- Sequential Monte Carlo: infer posterior distributions on the parameters from Bayes' theorem

Posterior

Likelihood

Prior

$$p(\text{parameters} \mid \text{data}) \propto p(\text{data} \mid \text{parameters})p(\text{parameters})$$

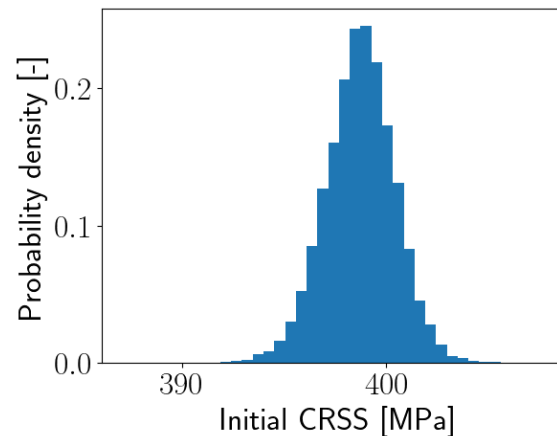
$$\text{stresses} = \mathcal{M}(m, g_0, H, g_0/g_1) + \mathcal{N}(0, \sigma_{std} = 5 \text{ MPa})$$

Predicted stresses from surrogate      Zero-mean Gaussian noise

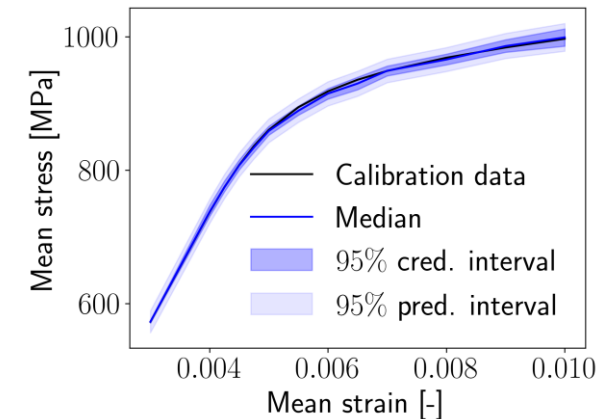
- Outputs to look at:

- Posterior distributions
- Maximum a posteriori (MAP) estimates and credible intervals
- Posterior predictive distribution
- Surrogate prediction with ground-truth parameter values

Example posterior



Example posterior predictive distribution

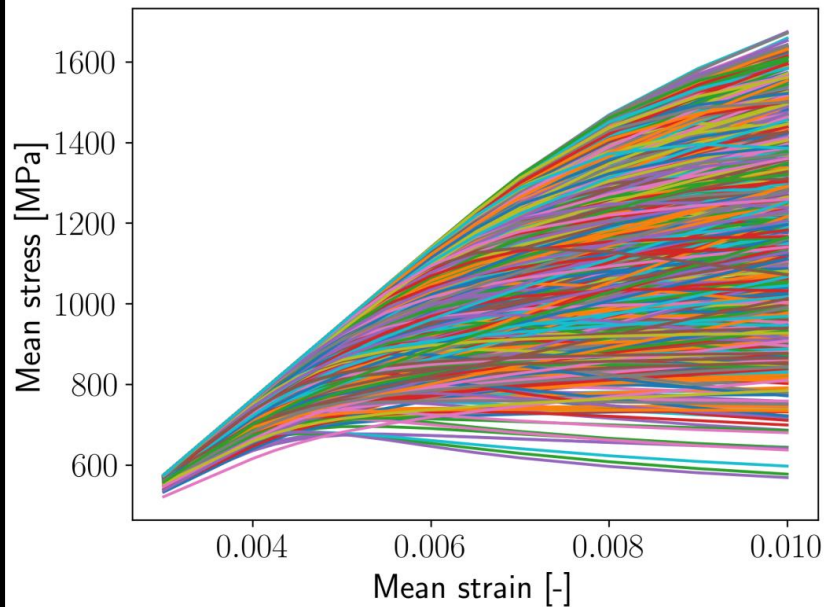


# Calibration approach



## Case 1: “Mean stresses only” calibration

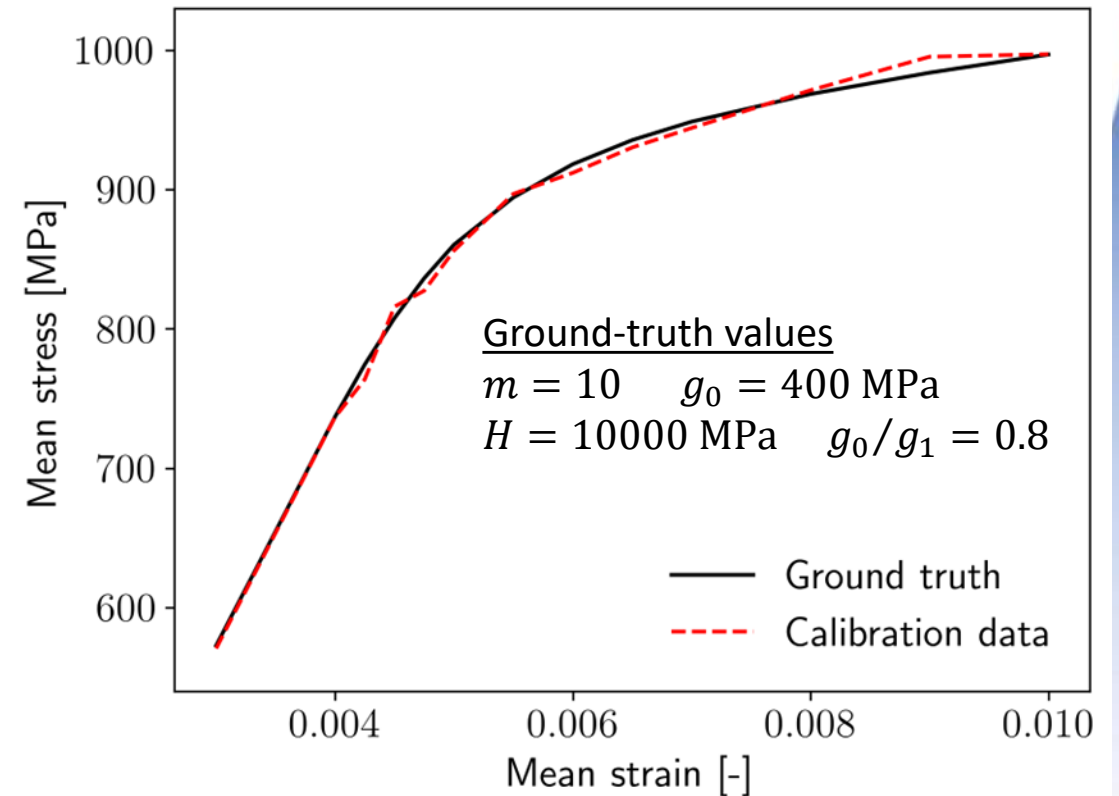
Train and test data



$$5 \leq m \leq 30$$
$$300 \text{ MPa} \leq g_0 \leq 700 \text{ MPa}$$
$$1000 \text{ MPa} \leq H \leq 30000 \text{ MPa}$$
$$0 \leq \frac{g_0}{g_1} \leq 1.5$$

Surrogate

Sequential Monte Carlo calibration

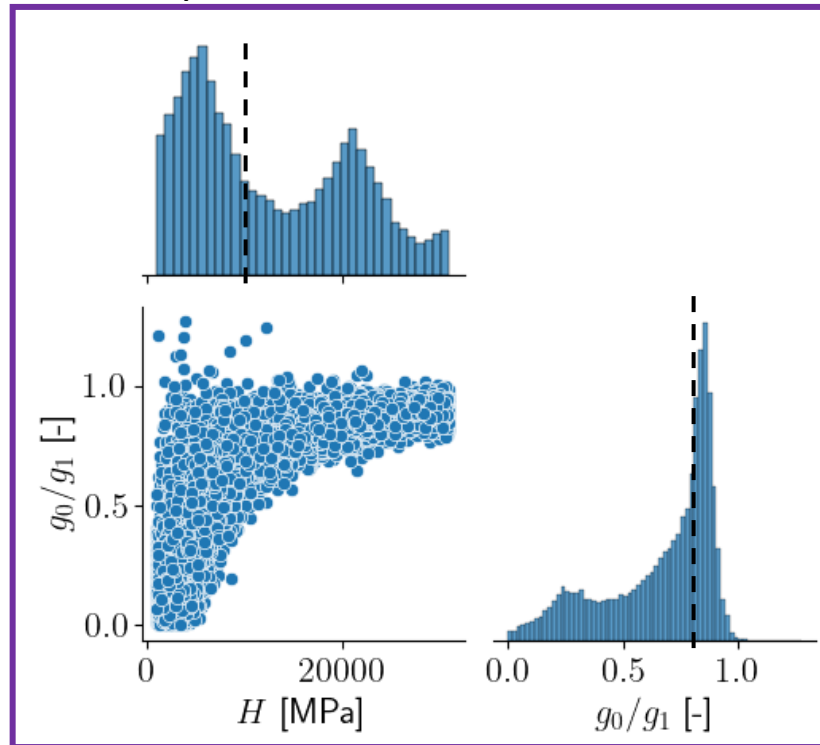
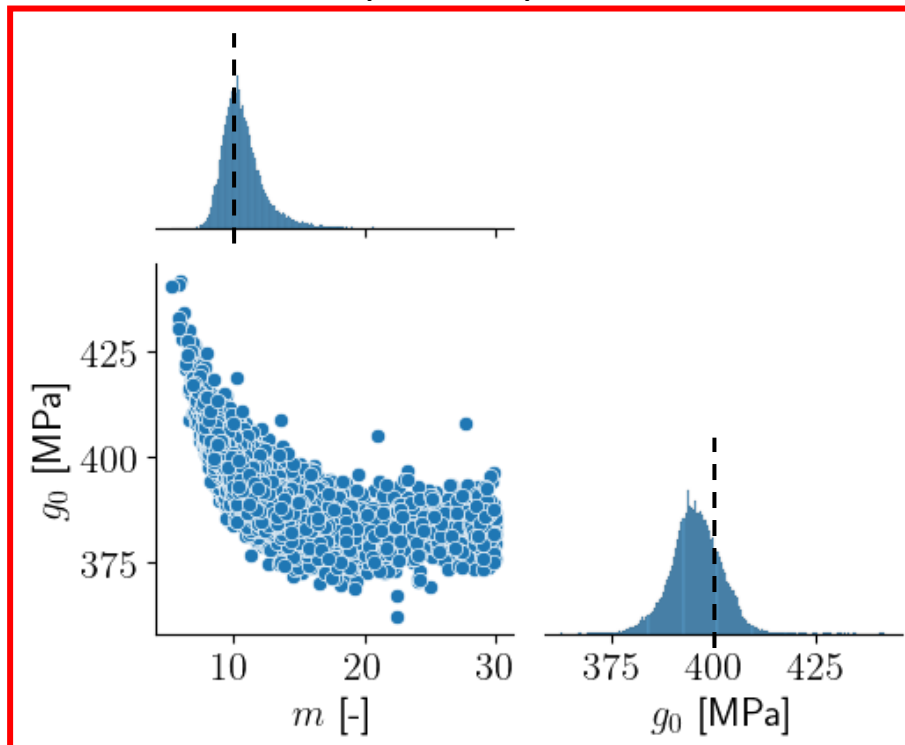


# Calibration results: Mean stresses only



- Rate sensitivity and initial CRSS are reasonably well calibrated
  - May be able to further reduce uncertainty
- Hardening parameters have identifiability challenges
  - Reasonable MAP, but posterior spans the entire parameter space except  $g_0/g_1 > 1$

Pair plots of posterior distributions for the parameters



Ground-truth values (- - -)

$m = 10$

$g_0 = 400$  MPa

$H = 10000$  MPa

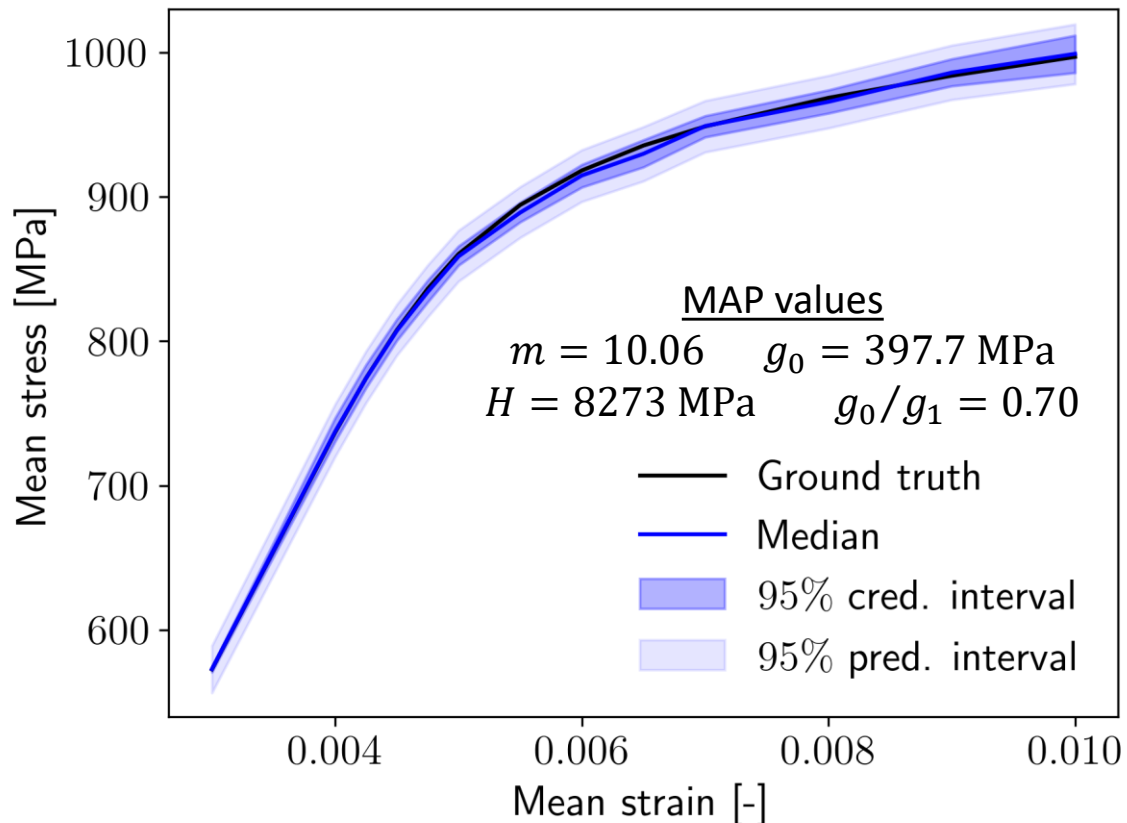
$g_0/g_1 = 0.8$



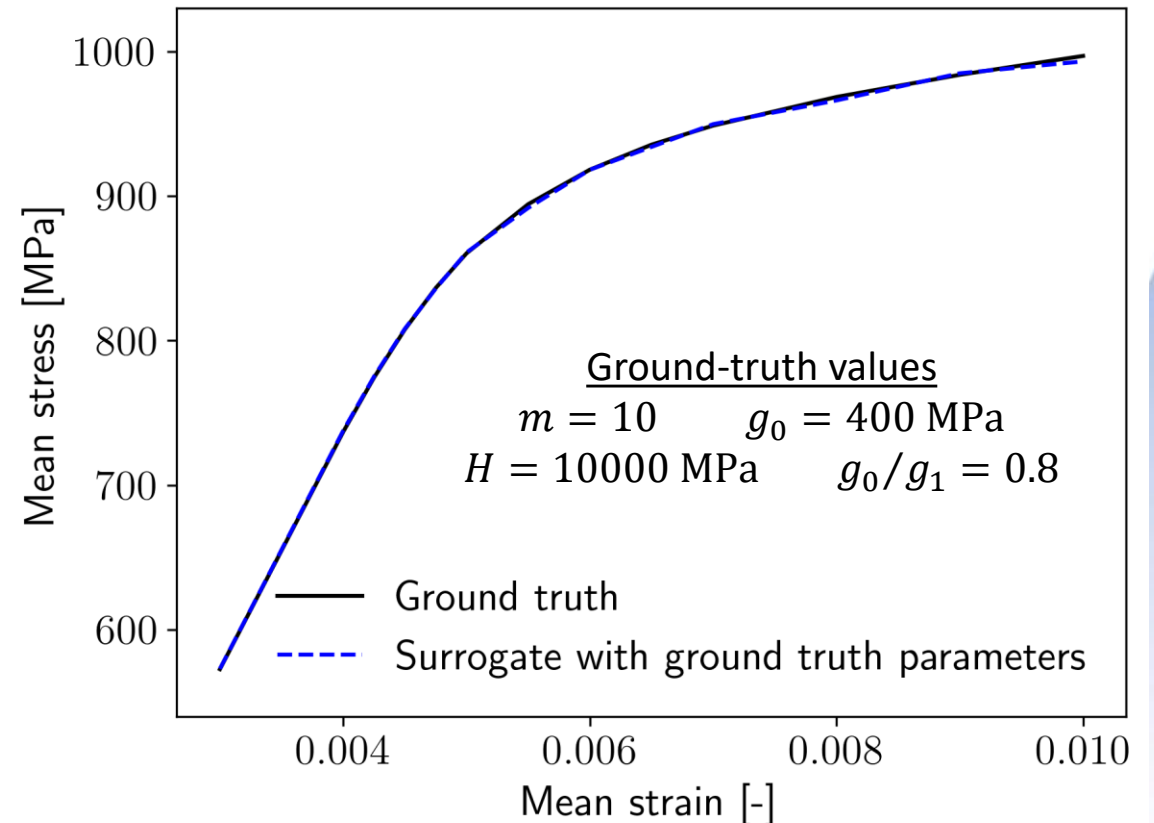
# Calibration results: Mean stresses only

- Posterior predictive distribution closely matches the data
- Surrogate prediction using the ground-truth parameters also closely matches the data
- Can grain-average stresses improve the calibration?

Posterior predictive distribution for the calibrated surrogate

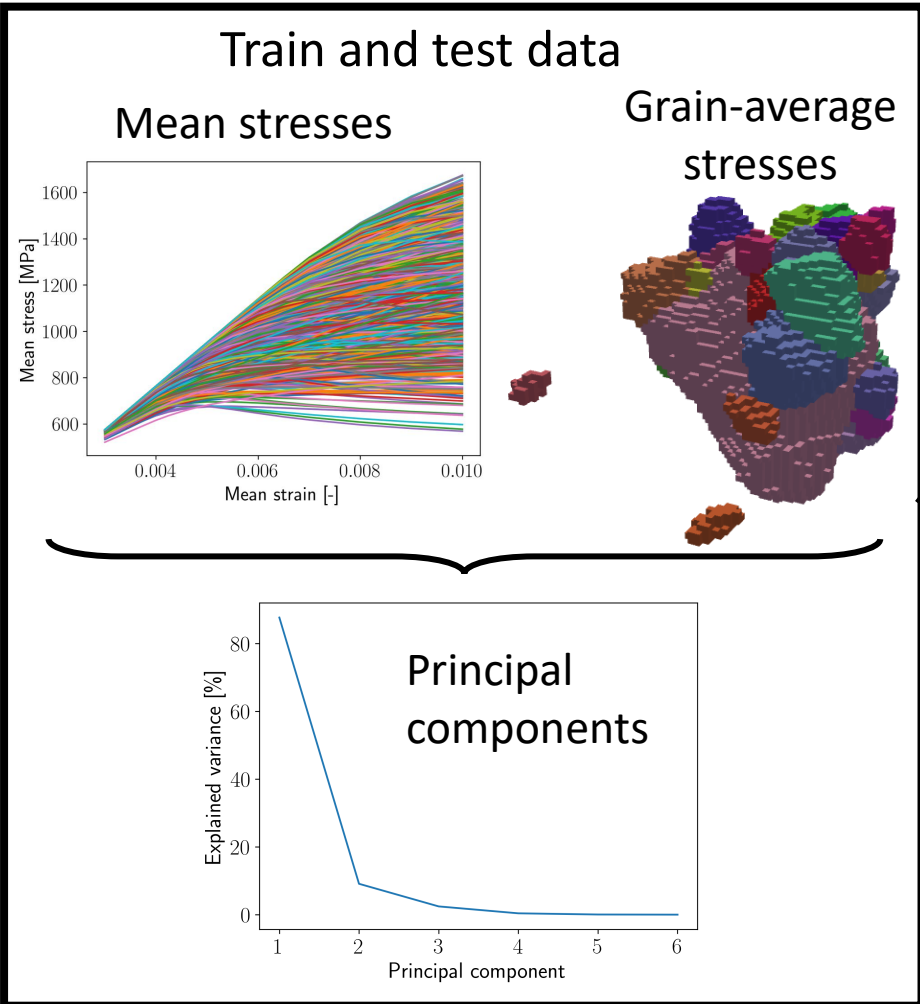


Surrogate prediction using ground-truth parameter values



# Calibration approach

Case 2: “Mean + grain stresses” calibration: use PCs for mean stresses and grain-average stresses



Sequential Monte Carlo calibration

Surrogate

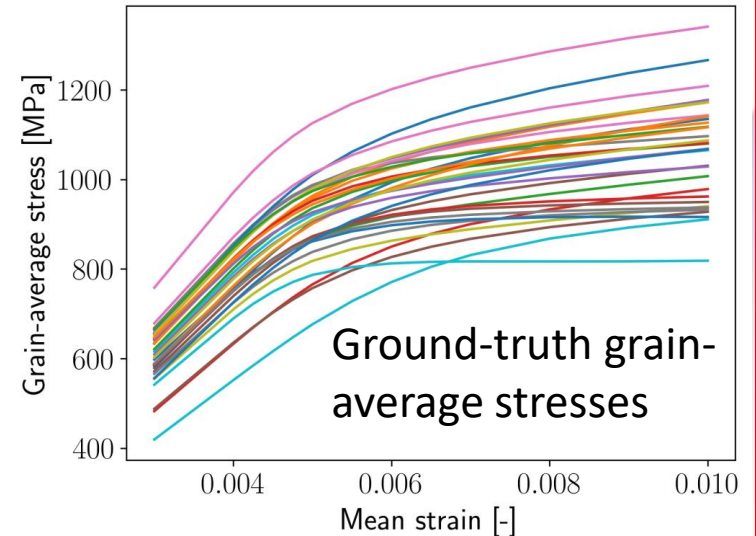
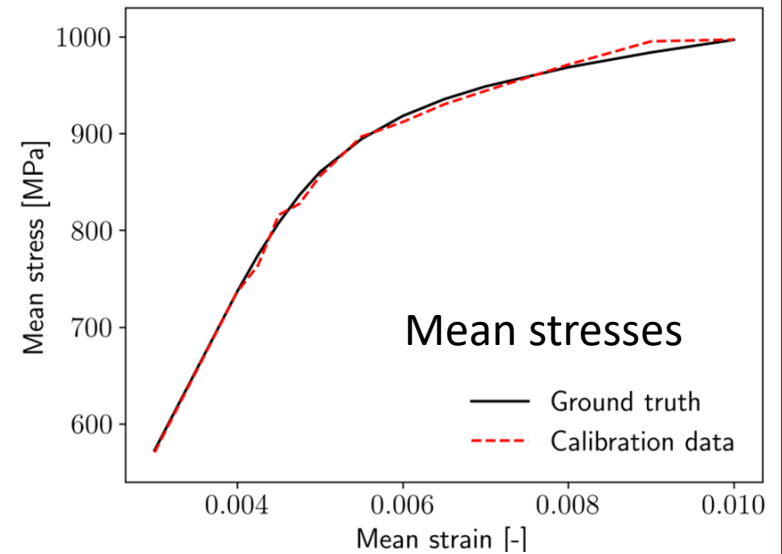
Ground-truth values

$$m = 10$$

$$g_0 = 400 \text{ MPa}$$

$$H = 10000 \text{ MPa}$$

$$g_0/g_1 = 0.8$$

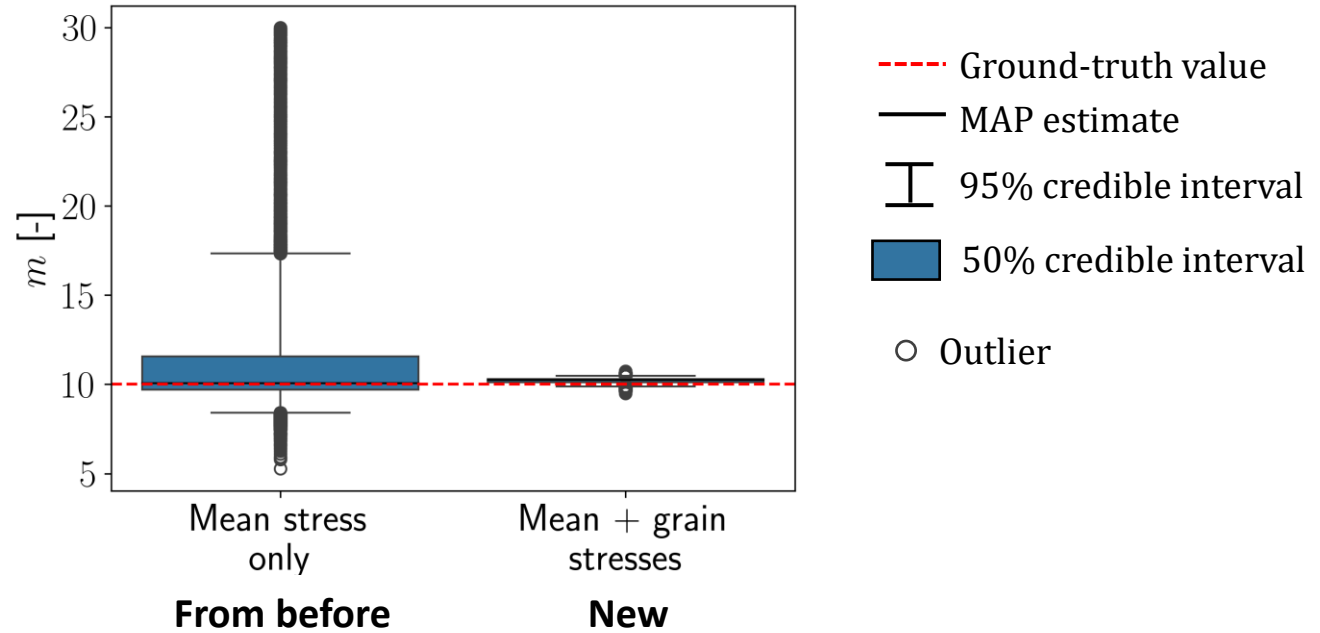


# Calibration results: Mean + grain stresses



- Compare marginal posterior distributions using box-and-whisker plots

Box-and-whisker plots for posterior distributions

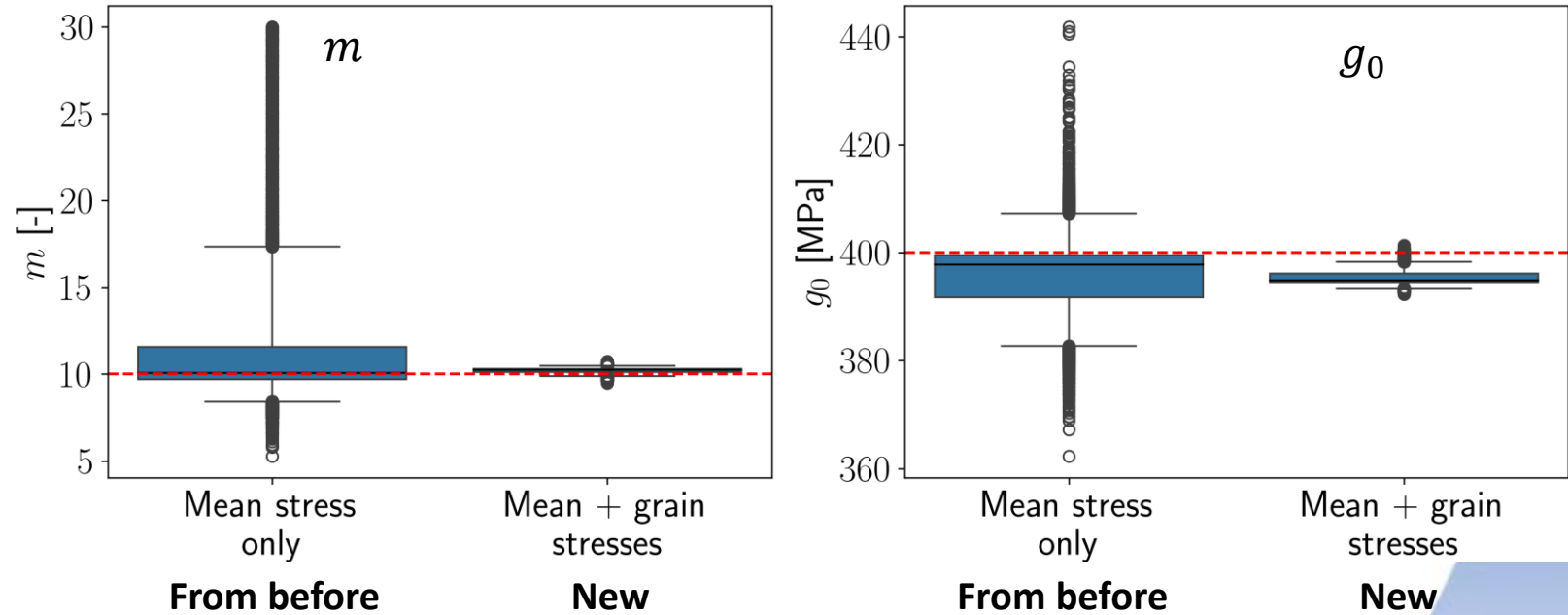


# Calibration results: Mean + grain stresses



- Compare marginal posterior distributions using box-and-whisker plots
- Rate sensitivity and initial CRSS: much tighter bounds
  - Likely need better resolution (in stress-strain curve and training data) to “perfectly” capture CRSS

Box-and-whisker plots for posterior distributions

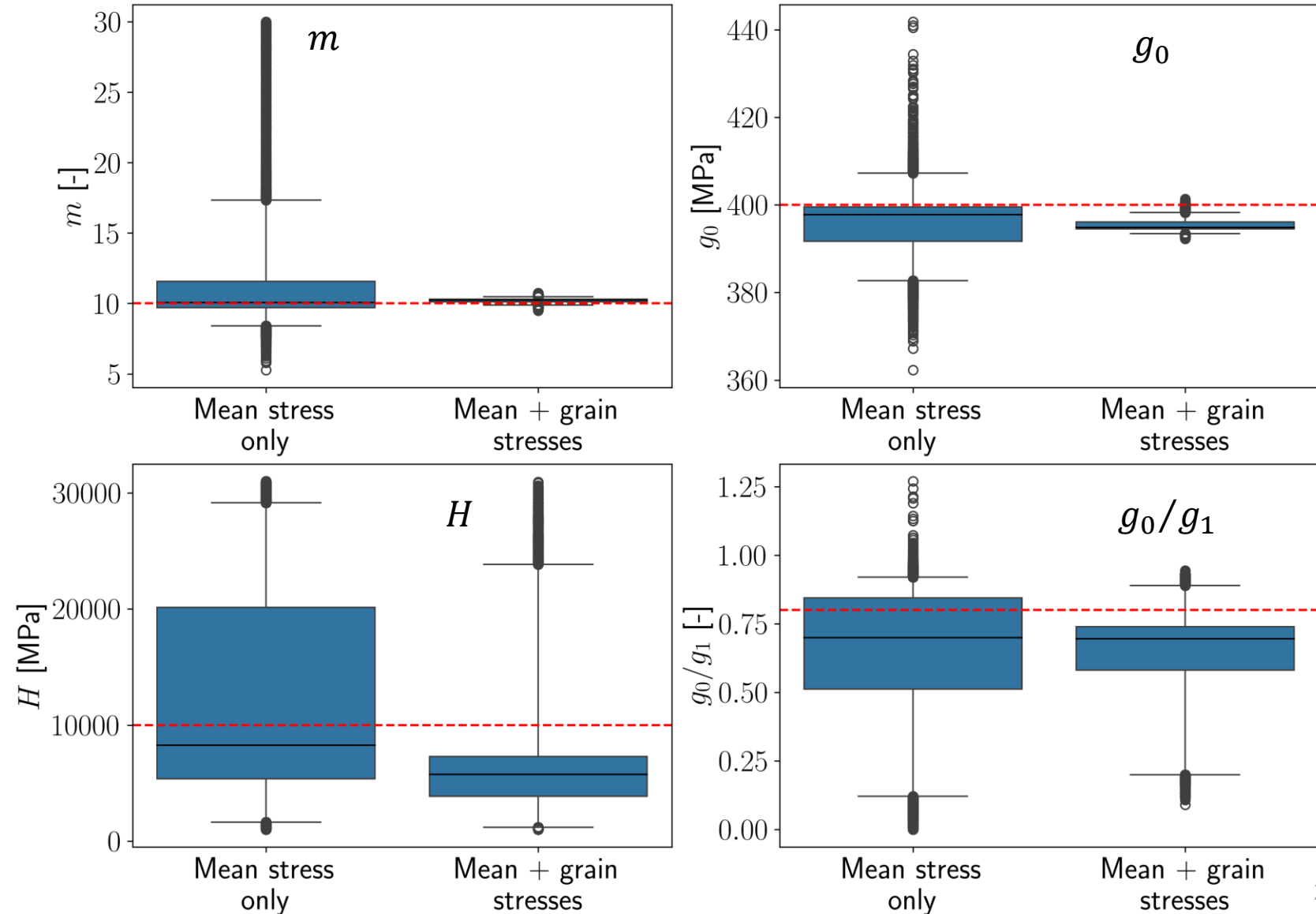


# Calibration results: Mean + grain stresses



- Compare marginal posterior distributions using box-and-whisker plots
- Rate sensitivity and initial CRSS: much tighter bounds
  - Likely need better resolution (in stress-strain curve and training data) to “perfectly” capture CRSS
- Hardening: some unrealistic values eliminated, but...
  - Some bias in the MAP predictions
  - Still significant uncertainty

Box-and-whisker plots for posterior distributions

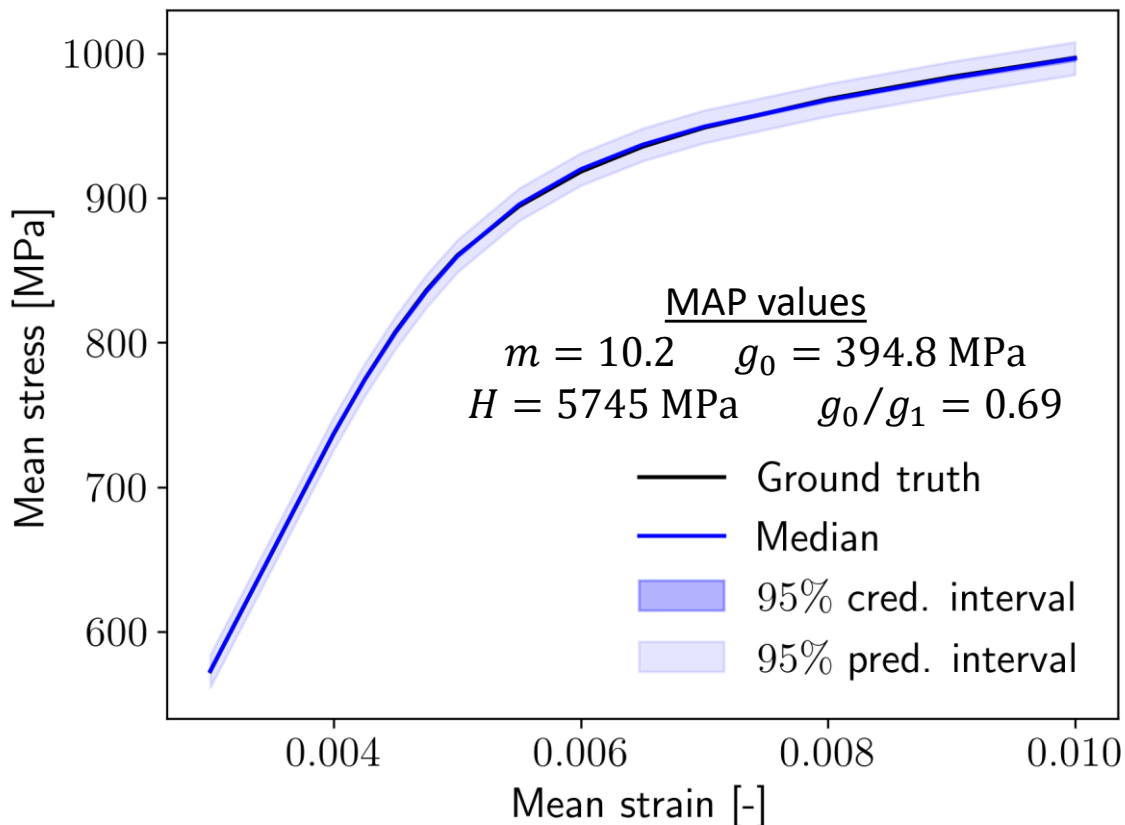


# Calibration results: Mean + grain stresses

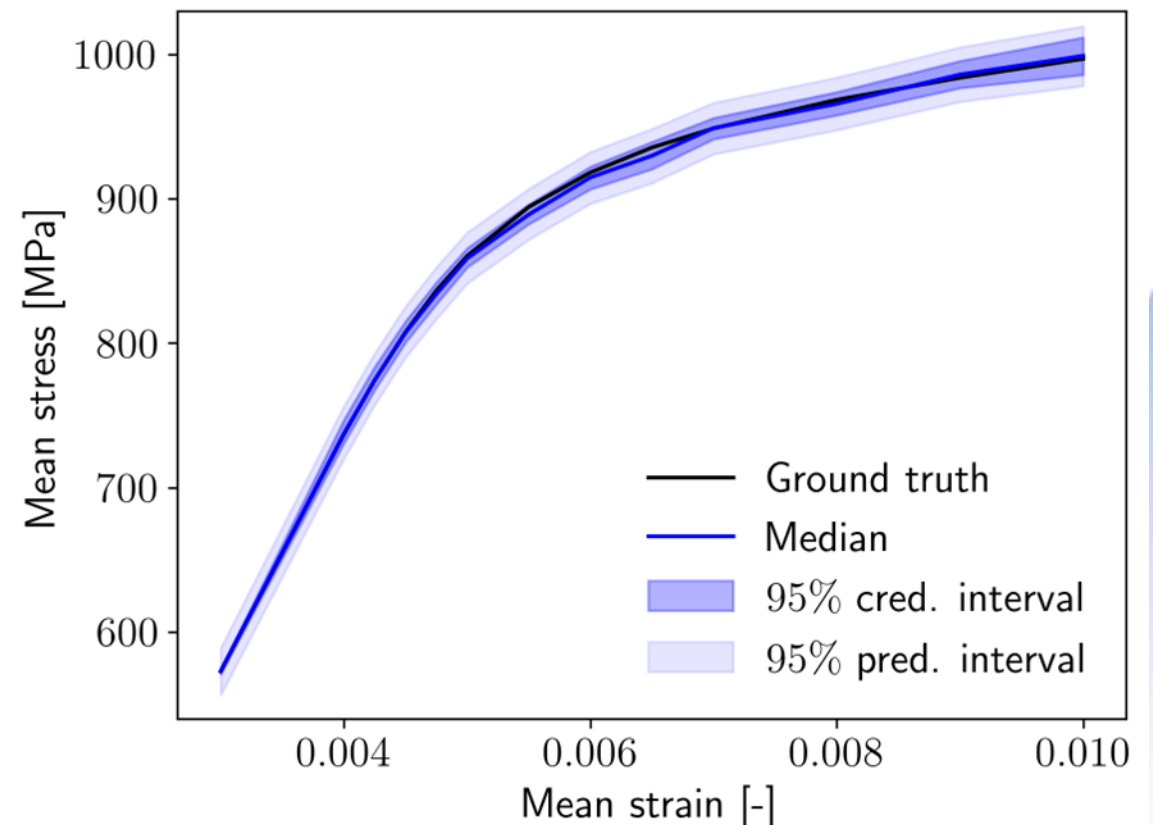


- **Posterior predictive distribution** closely matches the data
- Credible interval is smaller than before
  - Consistent with smaller credible intervals for the parameters

Surrogate calibrated with mean + grain stresses (**new**)



Surrogate calibrated with mean stresses only (**from before**)

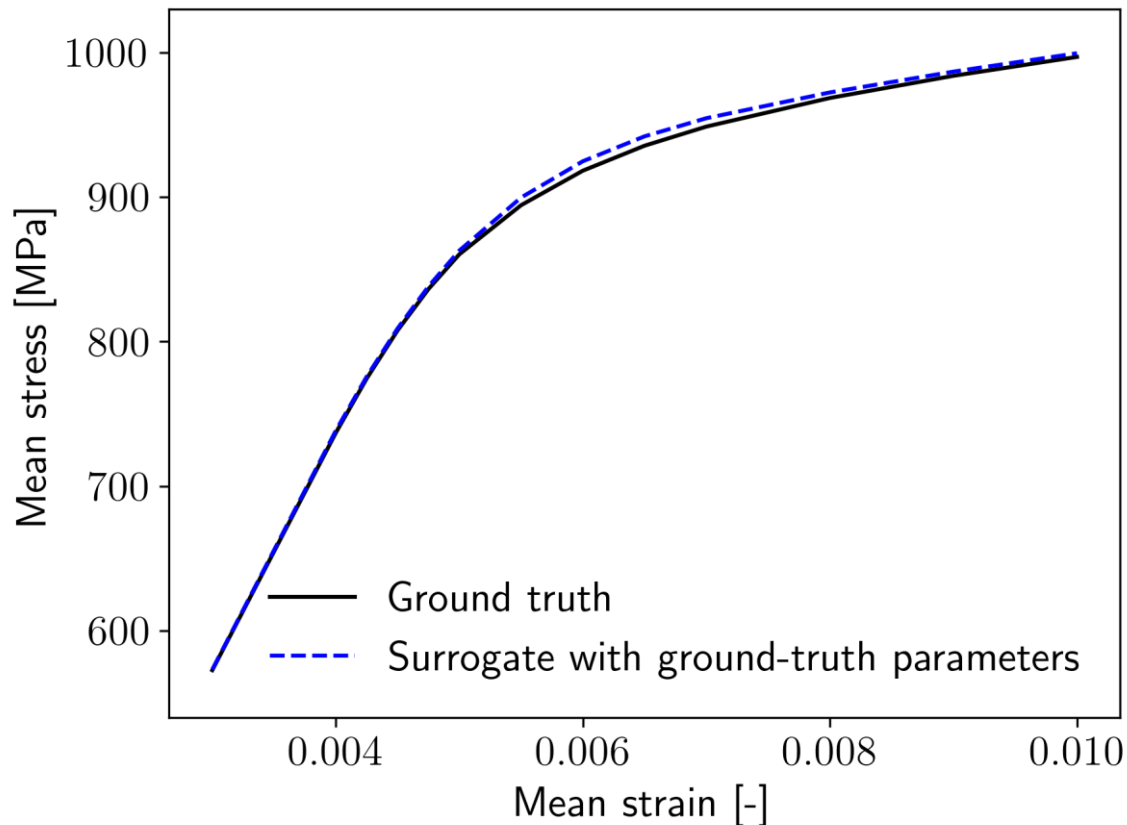


# Calibration results: Mean + grain stresses

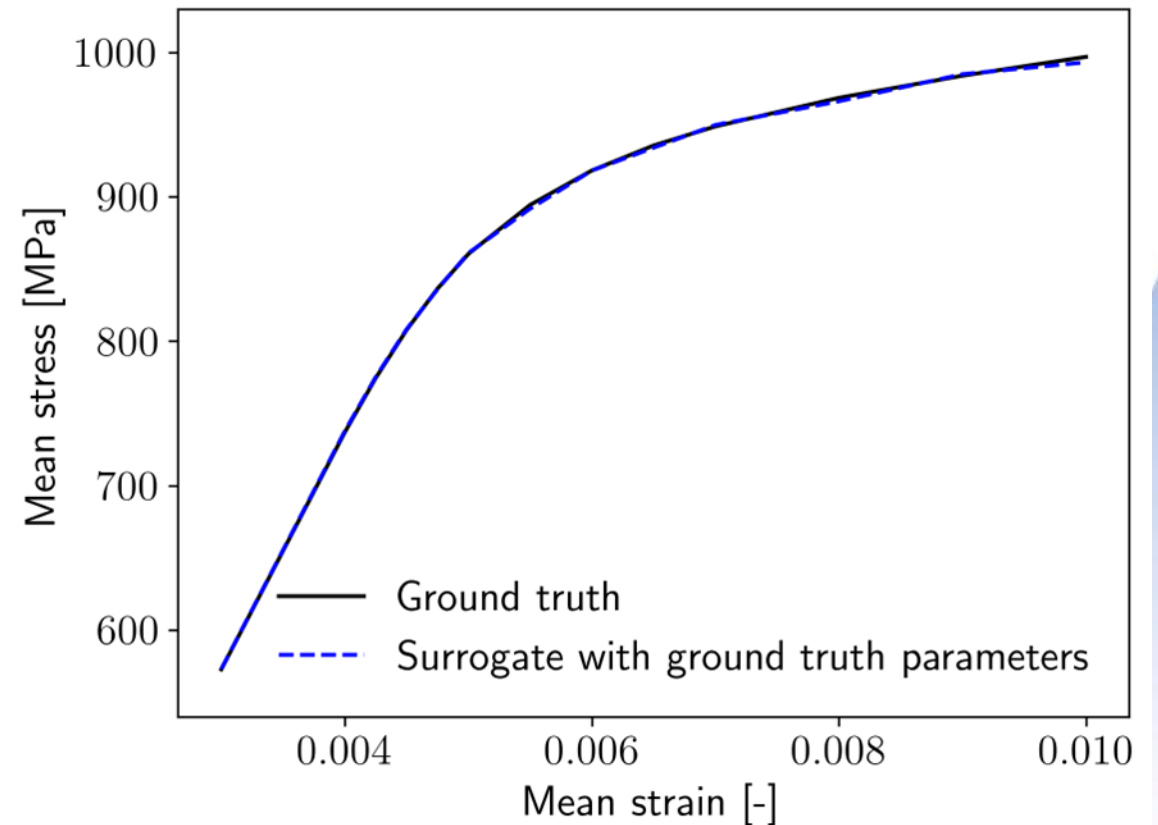


- The surrogate **with the ground-truth parameters** does not match the calibration data as well as before
- Adding more data may adversely impact surrogate accuracy

“Mean + grain stresses” surrogate prediction using ground-truth parameter values (**new**)



“Mean stresses only” surrogate prediction using ground-truth parameter values (**from before**)



# Conclusions and outlook

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- Probabilistic calibration recovers reasonable distributions for the calibration parameters
  - Better for rate sensitivity and initial CRSS; worse for hardening parameters
- Including grain-average stresses generally reduces uncertainty
  - Most effective for rate sensitivity and initial CRSS
  - Sensitive to surrogate model accuracy → need to balance this with the data being used
- Useful to examine uniqueness of hardening laws
  - Saturation-type laws (e.g., Voce) may have fewer problems
- Need to consider non-physical input parameter combinations
  - Here: excessive softening
- Dimensionality reduction (PCA): helpful for surrogate models and understanding how informative the data is
- SMC (embarrassingly parallelizable) + FFT crystal plasticity (~20 min/run) may be feasible calibration route (i.e., no surrogate model)
- Other interesting considerations...
  - Number of output data points, correlations between outputs for surrogate, crystal plasticity solver details/improvements, data from multiple strain rates, multi-step or multi-fidelity calibration, prior distributions

# Materialite codebase



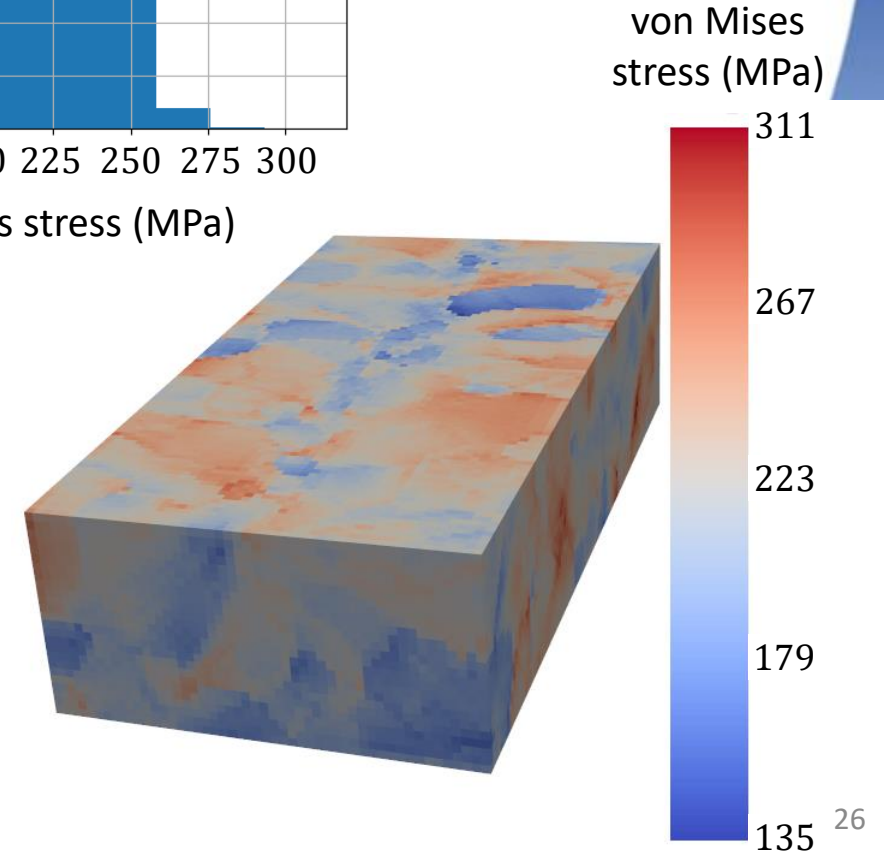
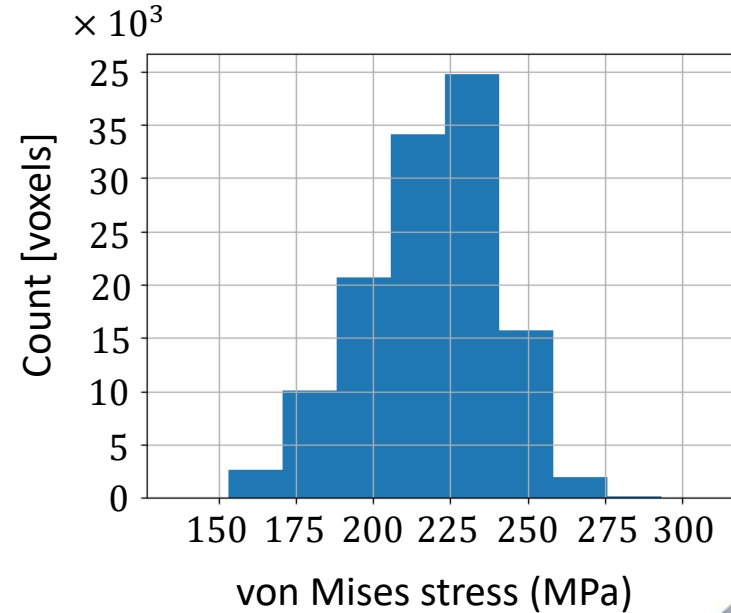
All simulations completed using the NASA Langley *Materialite* codebase

Core aspects of *Materialite* include:

- Ease of use
- Performative and state-of-the-art models
- Model chaining and interoperability
- Built in visualization and analysis capabilities

## Example model chain and visualization

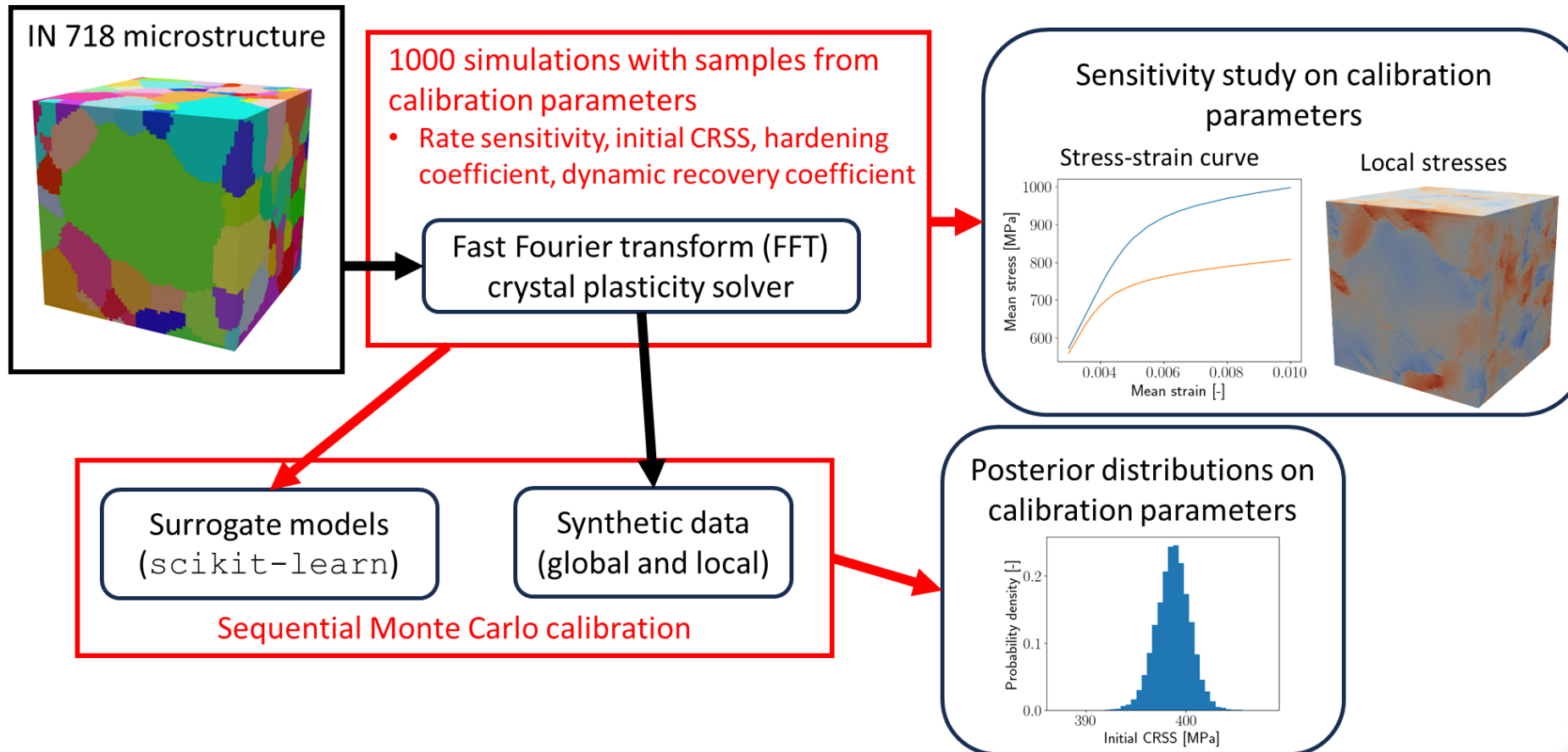
```
material.run(coarsening_model)
        .run(weld_model)
        .map_random_orientations()
        .run(mechanical_model)
material.plot("von_mises_stress")
material.fields["von_mises_stress"].hist()
```



# Acknowledgements



- This work was supported by the NASA Aeronautics Research Mission Directorate (ARMD) Transformational Tools and Technologies (TTT) project
- Contact information: [joshua.pribe@nasa.gov](mailto:joshua.pribe@nasa.gov)





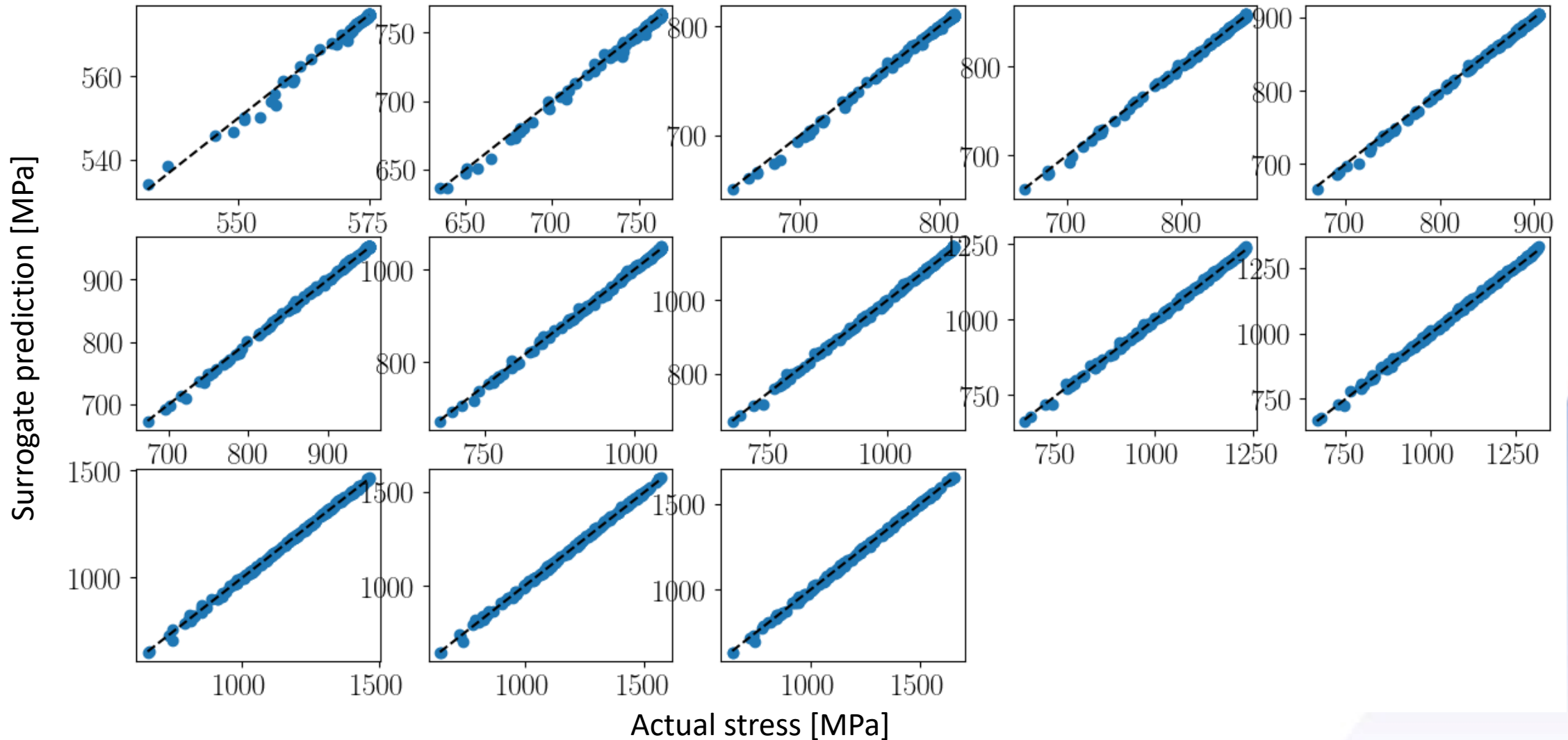
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# Backup slides

# Mean stresses surrogate model



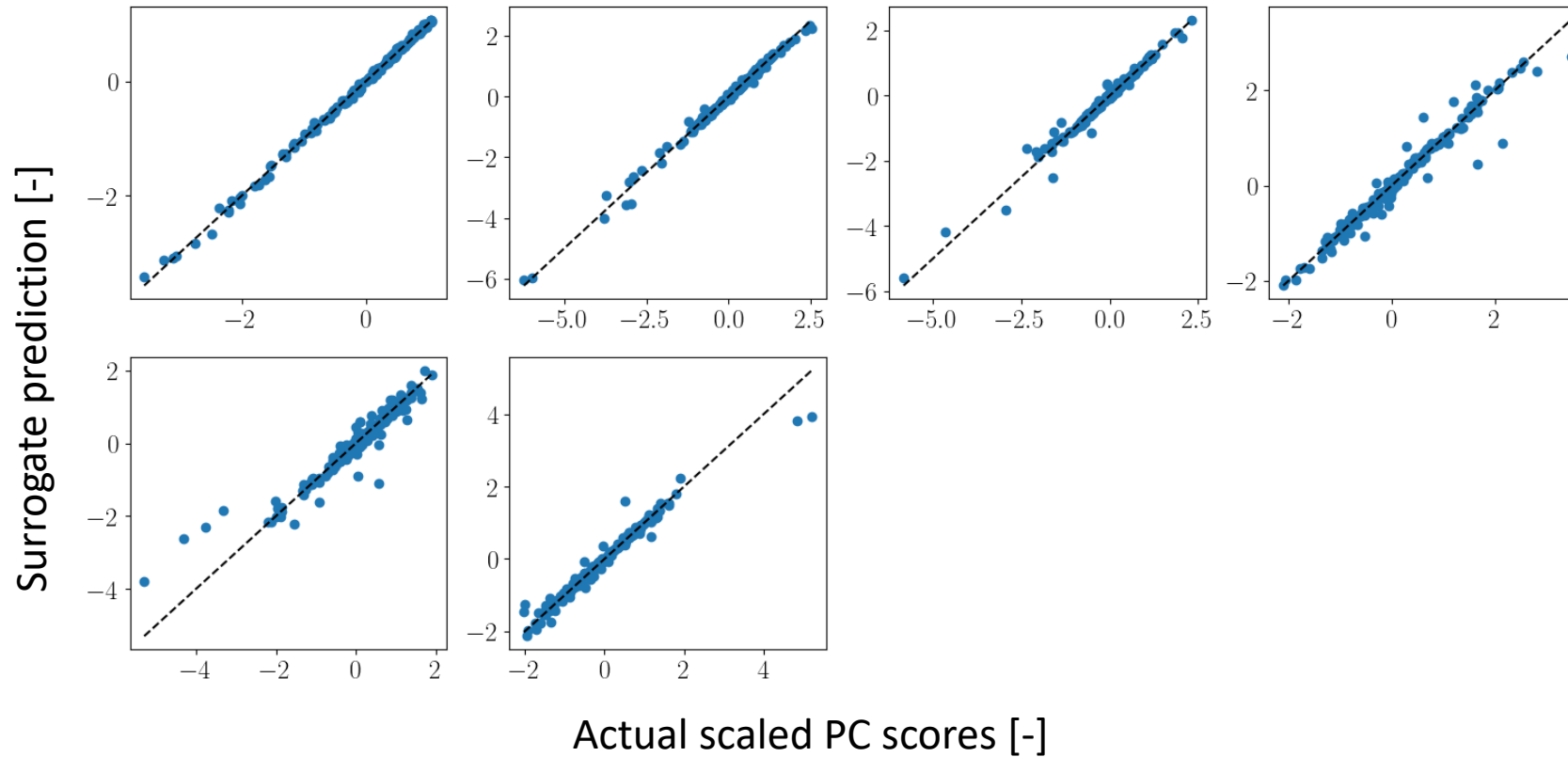
Surrogate performance on test set of mean stresses



# Mean + grain stresses surrogate model



Surrogate performance on test set of PCs for mean + grain stresses



# Crystal plasticity: Simulation methods

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- Based on open-source implementation of “Fourier-Galerkin” method<sup>1,2</sup>
  - Conjugate gradient solver for global iterations with same consistent tangent/Jacobian as in finite element methods
- Quadratic convergence rate for global and material iterations
- Direct enforcement of mixed “BCs”<sup>3</sup>
  - “Basic scheme”<sup>4</sup> and its variations<sup>5</sup> apply an on-the-fly correction to the strain rate
- Adaptive time step → substantial efficiency gains

<sup>1</sup>J. Zeman et al., A finite element perspective on nonlinear FFT-based micromechanical simulations, *Int J Numer Meth Engr* 111 (2017) 903–926. <https://doi.org/10.1002/nme.5481>.

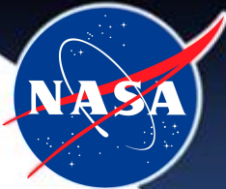
<sup>2</sup>T.W.J. de Geus et al., Finite strain FFT-based non-linear solvers made simple, *Comput Methods Appl Mech Eng* 318 (2017) 412–430. <https://doi.org/10.1016/j.cma.2016.12.032>.

<sup>3</sup>S. Lucarini, J. Segurado, An algorithm for stress and mixed control in Galerkin-based FFT homogenization, *International Journal for Numerical Methods in Engineering* 119 (2019) 797–805. <https://doi.org/10.1002/nme.6069>.

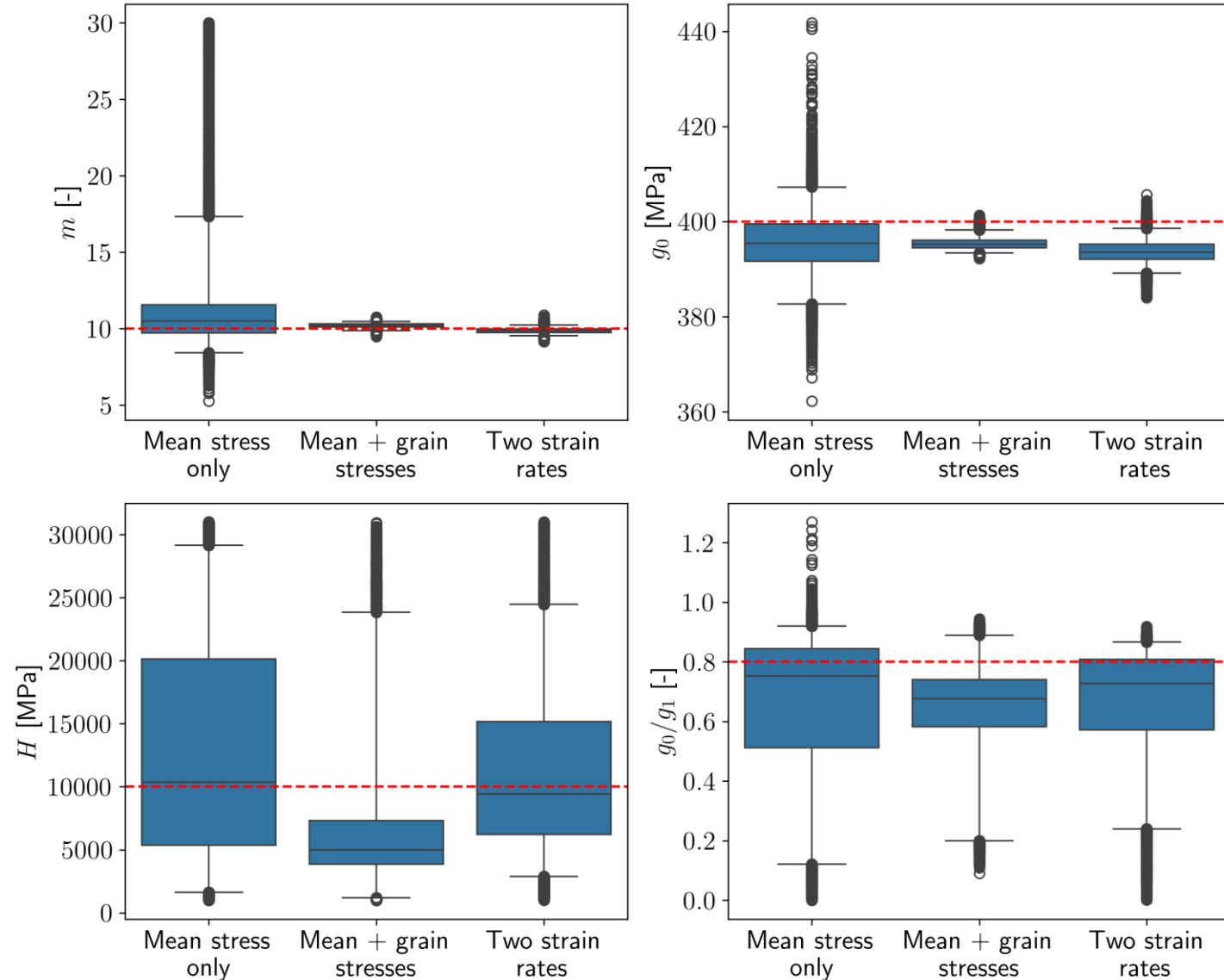
<sup>4</sup>H. Moulinec, P. Suquet, A numerical method for computing the overall response of nonlinear composites with complex microstructure, *Comput Methods Appl Mech Eng* 157 (1998) 69–94. [https://doi.org/10.1016/S0045-7825\(97\)00218-1](https://doi.org/10.1016/S0045-7825(97)00218-1).

<sup>5</sup>R.A. Lebensohn et al., An elasto-viscoplastic formulation based on fast Fourier transforms for the prediction of micromechanical fields in polycrystalline materials, *Int J Plast* 32–33 (2012) 59–69. <https://doi.org/10.1016/j.iijplas.2011.12.005>.

# Calibration results: Two strain rates



Calibration using mean stresses from synthetic experiments at two strain rates gives similar results to the “Mean + grain stresses” case

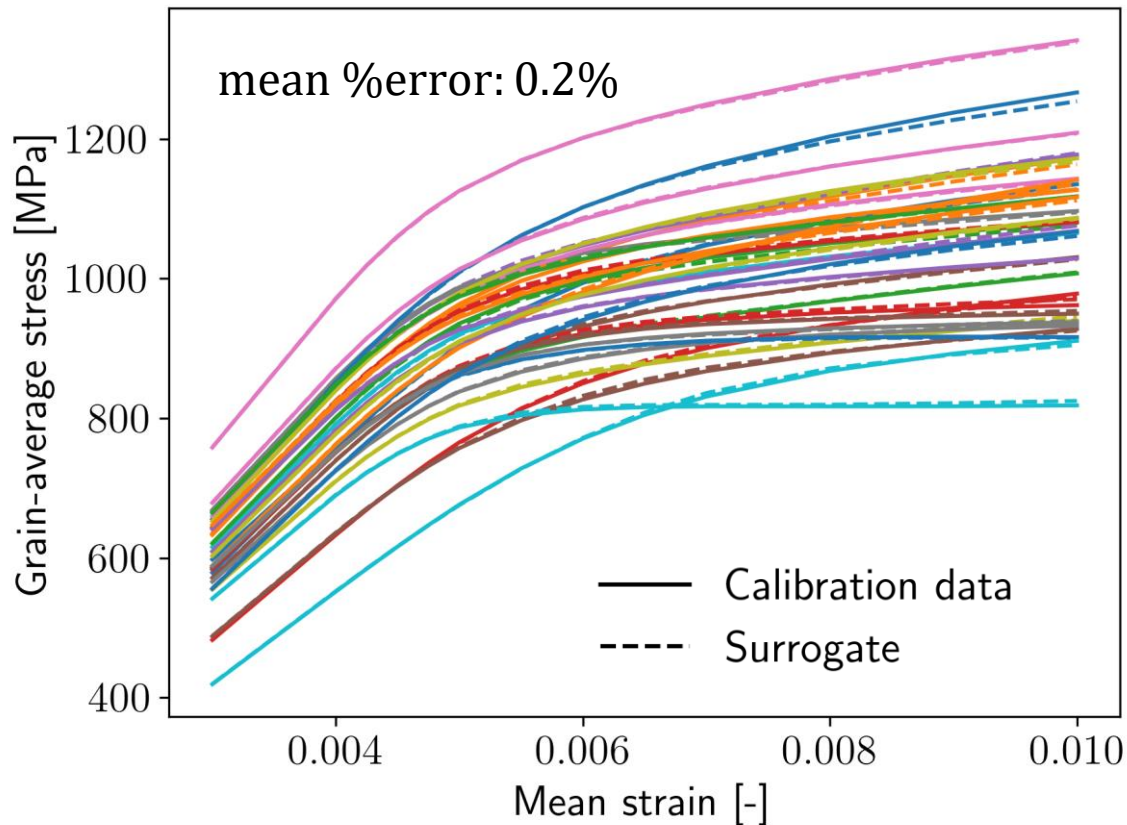


# Calibration results: Mean + grain stresses



- Uniqueness issues appear with the grain-average stresses too
- Difficult to get information about compliance of the grains in the plastic regime

Median predicted grain-average stresses from calibrated surrogate



Predicted grain-average stresses from surrogate with ground-truth parameter values

